TEXAS INSTRUMENTS

SOFTWARE

TI-95 CHEMICAL ENGINEERING LIBRARY

GUIDEBOOK

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GUIDEBOOK

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Table of Contents

This manual provides instructions for using the TI-95 Chemical Engineering cartridge. Before using this manual, you should already be familiar with the scientific-calculator functions, described in the *TI-95 User's Guide*.

Contents of This Guidebook

This guidebook describes the programs contained in the TI-95 Chemical Engineering cartridge. The book is organized to help you use the programs.

Organization of the Guidebook

The guidebook includes 12 chapters.

Chapter 1 covers the general use and care of the cartridge, provides information about using the programs, and describes how to use an optional printer with the programs.

Chapters 2 through 12 provide detailed information about each program in the cartridge. The discussion of each program includes:

- A brief presentation of general information about the program, the inputs required, and the equations used by the program.
- References to sources for the method and/or equations.
- Step-by-step instructions for using the program.
- An example demonstrating the use of the program.

Two appendixes are included at the end of the guidebook.

Appendix A contains a list showing the data registers used with each program. This is helpful when you need to find a register that is not used by the cartridge during a specific program. Appendix A also includes a list of all flags used in each program, and a table of the compounds whose properties are built into the cartridge.

Appendix B contains service and warranty information that may be useful in case of difficulty.

The Chemical Engineering Library is a group of 19 computer programs designed specifically for chemical engineers and chemical engineering students. The programs are based upon proven techniques of estimation, calculation, and design.

Preface

The selection of programs in the Chemical Engineering Library is intended to provide you with a complete physical property data bank and basic shortcut design methods for the primary unit operations. This library, along with your own programs for your TI-95, gives the capability for preliminary plant/process design for a wide variety of chemical engineering applications. For this reason, the unit operations programs were made as general as possible.

The most reliable methods, within the limits of simplicity, were chosen for the physical property estimation programs. Many of these methods are specific. (One, for example, deals with hydrocarbons only.) Therefore, the programs were tested for accuracy using a group of compounds with a variety of chemical characteristics. These compounds are:

benzene
1,3 butadiene
chloroform
cyclohexane
ethylene glycol
ethylene oxide
n-octane
propane
propanol
propylene
vinyl chloride

The accuracy figures reported in this manual for the physical property routines are based on data from *Physical Properties of Hydrocarbons and Related Compounds* by R. W. Gallant and *Tables on the Thermophysical Properties of Liquids and Gases* by N. B. Vargaftik. Individual property inaccuracies for a given compound or physical state may be considerably greater than the averages given, particularly for transport properties.

Chapter 1: Getting Started

This chapter describes the handling, installation, and use of the TI-95 Chemical Engineering cartridge. It also introduces you to the programs available on the cartridge.

Table of Contents

Installing the Chemical Engineering Cartridge

You should become familiar with the proper handling and installation of the Chemical Engineering cartridge before using the programs.

Handling the Cartridge

Handle the cartridge with the same care you would give any other electronic equipment.

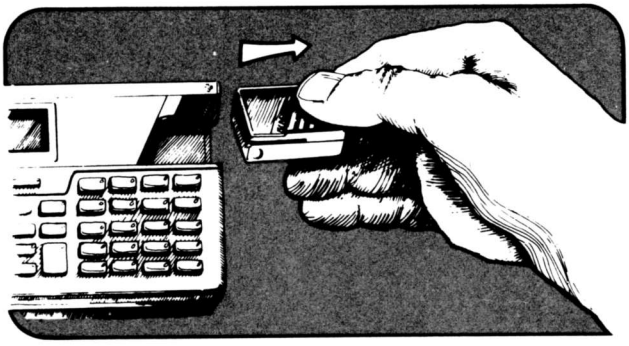
- Avoid static electricity. Before handling the cartridge, you should touch a metal object to discharge any static electricity.
- Store the cartridge in its original container or in the cartridge port on the upper right side of the TI-95.

Installing the Cartridge

The calculator is shipped with a port protector installed in the cartridge port. This protector resembles a cartridge and is installed to prevent dust from accumulating on the electrical contacts inside the port. (It is a good practice to always keep a cartridge or the port protector in the port.)

To install the Chemical Engineering cartridge:

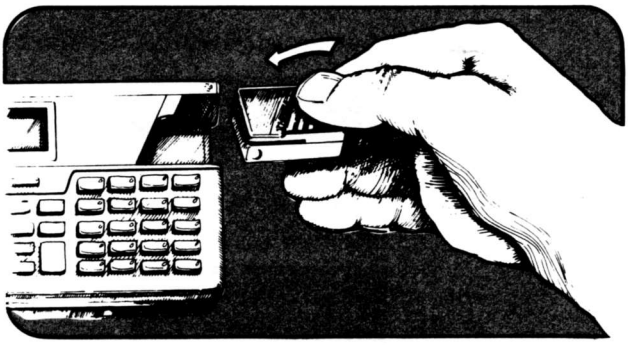
1. **Turn the calculator off.** Installing a cartridge while the TI-95 is on may result in memory loss.
2. If the port protector or another cartridge is already installed, remove it as shown below. Place your thumb on the ridged area at the top of the cartridge and slide it to the right.



After you remove a cartridge, be sure to store it properly.

Installing the Cartridge (Continued)

3. Turn the Chemical Engineering cartridge so that the ridges are facing upward and insert it into the port, small end first.



4. Slide the cartridge to the left until it snaps into place.

Displaying the Chemical Engineering Menu

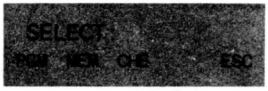
After installing the cartridge, you can then display the CHEM ENGINEERING menu. Each selection on this menu represents a different category of chemical engineering calculation. For each category, the cartridge contains a selection of programs.

Accessing the Chemical Engineering Cartridge

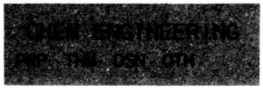
To access the cartridge and display the **CHEM ENGINEERING** menu:

1. Turn the calculator on and press [RUN].

   The calculator displays:



2. Press ⟨CHE⟩ to display the calculation categories in the cartridge.

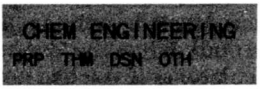


The Chemical Engineering Menu

The **CHEM ENGINEERING** menu, which is described on the following pages, enables you to select the type of chemical engineering calculation you want to perform. When you make a selection, the calculator displays another menu that lets you choose the specific program you want to run.

The Chemical Engineering Menu (Continued)

When you press [RUN] ⟨CHE⟩, the calculator displays the categories of chemical engineering calculations.



⟨PRP⟩ Displays a menu that lets you select from the following properties programs.

Properties Table
Gas Properties: Viscosity and Thermal Conductivity
Liquid Properties: Viscosity, Thermal Conductivity, and Density
Other Properties: Vapor Pressure and Raoult's Law K-Value, Critical Properties, and Latent Heat of Vaporization

⟨THM⟩ Displays a menu that lets you select from the following thermodynamics programs.

Soave-Redlich-Kwong Thermodynamics
Peng-Robinson Thermodynamics
Specific Heat

⟨DSN⟩ Displays a menu that lets you select from the following design programs.

Pipe Design for Liquid Flow
Absorber Design
Distillation Design
Heat Exchanger Design
Heat Transfer Coefficient Estimation

⟨OTH⟩ Displays a menu that lets you select from the programs that are not in the categories of properties, thermodynamics, or design. The following are the other programs in the library.

Equilibrium Flash Calculation
Activity Coefficient

Using a Cartridge Program

At any point in a program, you can stop using the program and start using the calculator's built-in functions. You do not need to press any special keys to exit the program. In some instances, however, you may want to return to the same program later or run another program.

Performing Calculations During a Program

Most of the time when you use a program, it is not actually running. When you press a key in the menu, the calculator responds by running a specific part of the program, indicated by **RUN** in the display (usually for a fraction of a second). When the **RUN** indicator is off, you can use the calculator as if you had not even selected a program.

During a program, you can perform calculations and not affect the progress of the program. Although some calculations cause the menu selections to change, you can still continue with the program at the same point from which you left it.

- If the program's menu selections are still in the display, you can proceed with the program by pressing the applicable key on the menu.
- If your calculations involved a function such as [CONV], which displays its own menu, you can restore the program menu by pressing the [OLD] key.

  Note: If you interrupt a program by running another program that redefines the function keys, you cannot use the [OLD] key to continue with the previous program. You also cannot continue with a program if the numbers in memory registers used by the program are altered during an interruption.

Interpreting Displayed Values

The programs identify every result or entry by including a label and = to the left of the number. Any value that appears without an identifying label is not important. Unlabeled values appear because the program used them in the display register before it stopped to display the menu. Do not consider unlabeled values to be results.

When You Want to Return to a Previous Menu

After you work through an option of the program, you can often return to the menu in which you select that option. Because the programs retain your entries for reuse, you can change only the entries you want to, and obtain the result without reentering the numbers that remain the same.

When you want to return to a menu displayed earlier in a program, press ⟨ESC⟩. The menu you return to may also have an ⟨ESC⟩ key, so sometimes you can press ⟨ESC⟩ more than once to reach an earlier menu. If no escape key is labeled, you can often press INV ⟨EOD⟩ or INV ⟨-->⟩ instead.

If no escape key is labeled and INV ⟨EOD⟩ or INV ⟨-->⟩ does not function as an escape, you can return to an earlier menu only by pressing RUN ⟨CHE⟩ and using the program until it reaches the desired menu.

When You Finish a Program

When you finish using a program, the last menu selections used by the program usually remain in the display. If you want to clear these selections, press 2nd [F:CLR] or turn off the calculator. You can also replace the selections with another menu such as the menu generated by pressing [NUM] or [CONV].

When You Want to Run Another Program

When you want to stop using a program and run another one, use one of the methods given below.

- If you want to run another program and there is not a way for ⟨ESC⟩ to return to the appropriate menu, press RUN ⟨CHE⟩ to display the **CHEM ENGINEERING** menu. Then select the new program.

- If you select a program and decide it is not the program you intended, but the program you want is in the same category, you can press ⟨ESC⟩ to return to the menu that lets you select other programs.

Entering the Physical Parameters of a Compound

Most of the programs in the Chemical Engineering library perform calculations based on one or more physical parameters of a compound. You have a choice of methods for entering the required physical parameters.

Ways You Can Supply Physical Parameters

The chemical engineering library has a built-in table of physical parameters for 261 of the more popular industrial compounds. The programs can also work with a compound that is not in the table.

- If your compound is in the table, identify it by compound number. The program generates the available parameters without your having to enter them individually. When the program presents the menu of physical parameters for you to check, you can usually proceed with the program, accepting the generated values.
- If your compound is not in the table, specify that your compound is unlisted. When the program presents the menu of physical parameters for you to check, enter the values for all the parameters in the menu.

The table of compounds appears listed alphabetically on page 1-11 and listed numerically in Appendix A.

Indications that You are to Specify a Compound

When a program requires the physical parameters of a compound, it prompts you in either of two ways to specify the compound.

- The program deals with a pure substance, in which case it labels a function key as <#>.
- The program deals with a mixture, in which case it displays #(1) for the first component and labels a function key as <ENT> (the entry prompts for the other components are numbered accordingly).

Entering the Physical Parameters of a Listed Compound

If your compound is among those listed, enter its physical parameters as follows.

1. Find the number of your compound in the list of compounds.
2. Enter the number of the compound and press the appropriate key (<#> or <ENT>).

Entering the Physical Parameters of a Listed Compound (Continued)

3. When the program presents a menu of the physical parameters, you can check that the generated values are satisfactory. To display the value of a physical parameter, press [INV] and the key that corresponds to that parameter.

   Note: If you intend to display a value but forget to press [INV], whatever number is in the display register when you press the corresponding key replaces the value. In this situation, you probably should start over from the beginning of the program if you do not know the value for that physical parameter.

4. Decide whether to change any of the generated values.

   - If all the values are satisfactory, press ⟨EOD⟩ to accept them and proceed with the program. The initials EOD stand for End Of Data.

   - If you prefer a different value for any specific physical parameter, enter the value for that parameter and press the key that corresponds to the parameter. When all the physical parameters on the menu are satisfactory, press ⟨EOD⟩.

Example

You are running a program that requires the critical pressure, critical temperature, and boiling temperature of acetone (compound number 211). When the program prompts you to enter the number of the compound, enter **211** and press ⟨#⟩.

When the menu containing ⟨Pc⟩, ⟨tc⟩, and ⟨tb⟩ is displayed,
pressing [INV] ⟨Pc⟩ displays **Pc= 46.4**,
pressing [INV] ⟨tc⟩ displays **tc= 234.95**, and
pressing [INV] ⟨tb⟩ displays **tb= 56.25**. If these values are satisfactory, press ⟨EOD⟩ to proceed with the program.

Entering the Physical Parameters of an Unlisted Compound

If your compound is not in the list, enter the physical parameters as follows.

1. Enter a zero for the compound number and press the appropriate key (⟨#⟩ or ⟨ENT⟩) to specify that the compound is unlisted. The program assigns a value of zero to all the required physical parameters.

2. When the program presents a menu of the physical parameters, enter the value for each parameter shown on the menu.

   If you enter an incorrect value, enter the correct value before proceeding with the program.

3. When you have entered all the physical parameters correctly, press ⟨EOD⟩.

Example

You are running a program that requires the boiling temperature of fluoroacetone (tb = 75 °C). When the program prompts you to enter the number of the compound, enter **0** and press ⟨#⟩.

When the menu containing ⟨tb⟩ is displayed, pressing [INV] ⟨tb⟩ displays **tb = 0**. Enter 75 and press ⟨tb⟩ to enter the boiling temperature. To proceed with the program, press ⟨EOD⟩.

Alphabetical List of Compounds

The following list provides the number that identifies any compound that is included in the built-in table of properties. The five compounds that are marked with * do not have all the data for the compound. Their specific heat coefficients are stored as zero.

Compound Name	Number
A	
acetaldehyde	208
acetic acid	201
anhydride acetic acid (acetic anhydride)	258
butyl ester acetic acid (*n*-butyl acetate)	225
ethyl ester acetic acid (ethyl acetate)	223
methyl ester acetic acid (methyl acetate)	221
propyl ester acetic acid (*n*-propyl acetate)	224
acetone	211
acetonitrile	249
acetyl chloride	160
acetylene	127
dimethylacetylene	130
ethylacetylene	129
methylacetylene	128
acrolein	254
acrylic acid	206
ethyl ester acrylic acid (ethyl acrylate)	231
methyl ester acrylic acid (methyl acrylate)	230
allyl chloride	157
aniline	243
N,N-dimethylaniline *	247
B	
benzene	132
bromobenzene	169
n-butylbenzene	143

Compound Name	Number
B (continued)	
chlorobenzene	167
fluorobenzene	168
hexafluorobenzene	171
iodobenzene	170
1-methyl-2-ethylbenzene	140
1-methyl-3-ethylbenzene	141
1-methyl-4-ethylbenzene	142
n-propylbenzene	138
biphenyl	145
1,2-butadiene	87
3-methyl 1,2-butadiene	92
1,3-butadiene	88
n-butane	4
i-butane	5
2,2-dimethylbutane	12
2,3-dimethylbutane	13
2,2,3,3-tetramethylbutane	22
2,2,3-trimethylbutane	15
n-butanol	184
isobutanol	185
sec-butanol	186
tert-butanol	187
1-butene	52
isobutene	55
2,3-dimethyl 1-butene	72
3,3-dimethyl 1-butene	73
2-methyl 1-butene	59
3-methyl 1-butene	60
cis 2-butene	53
trans 2-butene	54
2,3-dimethyl 2-butene	74
2-methyl 2-butene	61

(continued)

Compound Name	Number
B (continued)	
n-butyl amine	239
isobutyl amine	240
n-butyraldehyde	210
butyric acid	203
methyl ester butyric acid (methyl *n*-butyrate) *	228
isobutyric acid	204
butyronitrile	251
C	
cumene	139
cyclobutane	95
cyclohexane	113
n-butylcyclohexane	124
1,1-dimethylcyclohexane	116
cis 1,2-dimethyl-cyclohexane	117
trans 1,2-dimethyl-cyclohexane	118
cis 1,3-dimethyl-cyclohexane	119
trans 1,3-dimethyl-cyclohexane	120
cis 1,4-dimethyl-cyclohexane	121
trans 1,4-dimethyl-cyclohexane	122
ethylcyclohexane	115
methylcyclohexane	114
cyclohexanol	192
n-propylcyclohexane	123
cyclohexene	126

Compound Name	Number
C (continued)	
cyclopentane	96
1,1-dimethylcyclopentane	99
cis 1,2-dimethyl-cyclopentane	100
trans 1,2-dimethyl-cyclopentane	101
ethylcyclopentane	98
methylcyclopentane	97
n-decylcyclopentane	107
n-dodecylcyclopentane	108
n-heptylcyclopentane	104
n-hexadecylcyclopentane	112
n-hexylcyclopentane	103
n-nonylcyclopentane	106
n-octylcyclopentane	105
n-pentadecylcyclopentane	111
n-propylcyclopentane	102
n-tetradecylcyclopentane	110
n-tridecylcyclopentane	109
cyclopentene	125
cyclopropane	94
D	
n-decane	39
1-decanol	193
1-decene	78
dibutyl amine	248
diethyl amine	241
diethyl ether	217
diethyl ketone	213
diethylene glycol	195
dimethyl amine	233

Compound Name	Number
D (continued)	
dimethyl ether	215
dimethyl sulfide	261
1,4-dioxane	257
diphenyl	145
dipropyl amine	244
n-dodecane	41
1-dodecene	80
E	
n-eicosane	49
ethane	2
chloroethane	153
1,1-dichloroethane	154
1,2-dichloroethane	155
1,2-dichloro-1,1,2,2-tetrafluoroethane (R114)	178
1,1,2-trichloroethane	156
1,1,2-trichloro-1,2,2-trifluoroethane (R113)	177
trichloroethylene	151
ethanol	181
ethyl amine	234
ethylbenzene	134
ethyl bromide	166
ethylene	50
perchloroethylene	152
ethylenediamine	235
1,1-difluoroethylene	164
ethylene glycol	194
ethylene imine	253
ethylene oxide	198
ethyl mercaptan	260

Compound Name	Number
F	
formaldehyde	207
formic acid	200
ethyl ester formic acid (ethyl formate)	219
methyl ester formic acid (methyl formate)	218
propyl ester formic acid (*n*-propyl formate)	220
furan	255
G	
glycerine	197
H	
n-heptadecane	46
2-methylheptane	23
3-methylheptane	24
4-methylheptane	25
n-heptane	14
1-heptanol	190
1-heptene	75
n-hexadecane	45
1-hexadecene	84
n-hexane	9
2,2-dimethylhexane	27
2,3-dimethylhexane	28
2,4-dimethylhexane	29
2,5-dimethylhexane	30
3,3-dimethylhexane	31
3,4-dimethylhexane	32
3-ethylhexane	26
3-methylhexane	16
2,2,5-trimethylhexane	38

(continued)

Compound Name	Number
H (continued)	
1-hexanol	189
1-hexene	62
cis 2-hexene	63
trans 2-hexene	64
cis 3-hexene	65
trans 3-hexene	66
I	
isoprene	93
M	
methane	1
chlorodifluoro-methane (R22)	176
chlorotrifluoro-methane (R13)	174
dichlorodifluoro-methane (R12)	173
dichloromonofluoro-methane (R21)	175
nitromethane	252
tetrachloromethane (carbon tetrachloride)	149
tetrafluoromethane (carbon tetrafluoride) (R14)	162
trichloromethane (chloroform)	148
trichlorofluoromethane (R11)	172
trifluorobromomethane	179
methanol	180
methyl amine	232

Compound Name	Number
M (continued)	
methyl bromide	165
methyl isobutyl ketone	214
methyl isobutyrate *	229
methyl chloride	146
methyl ethyl ether	216
methyl ethyl ketone	212
methyl fluoride	161
methyl mercaptan	259
methylene chloride	147
methylphenyl amine *	246
N	
neopentane	8
n-nonadecane	48
n-nonane	37
1-nonene	77
O	
n-octadecane	47
1-octadecene	85
n-octane	21
1-octene	76
P	
n-pentadecane	44
1-pentadecene	83
1,2-pentadiene	89
trans 1,3-pentadiene	90
1,4-pentadiene	91
n-pentane	6
i-pentane	7
3,3-dimethylpentane	20
2,3-dimethylpentane	18

Compound Name	Number
P (continued)	
2,4-dimethylpentane	19
3-ethylpentane	17
2-methylpentane	10
2-methyl–3-ethylpentane	33
3-methylpentane	11
3-methyl–3-ethylpentane	34
2,3,3-trimethylpentane	35
2,3,4-trimethylpentane	36
1-pentanol	188
1-pentene	56
cis 2-pentene	57
trans 2-pentene	58
2-methyl 2-pentene	67
cis 3-methyl 2-pentene	68
trans 3-methyl 2-pentene	69
cis 4-methyl 2-pentene	70
trans 4-methyl 2-pentene	71
1-pentyne	131
phosgene	159
propadiene	86
propane	3
1,2-dichloropropane	158
n-propanol	182
isopropanol	183
2-propanol	191
propionaldehyde	209
propionic acid	202
ethyl ester propionic acid (ethyl propionate)	227
methyl ester propionic acid (methyl propionate)	226
propionitrile	250
n-propyl amine	236
isopropyl amine	237

Compound Name	Number
P (continued)	
propylene	51
propylene glycol (1,2-propanediol)	196
propylene oxide	199
pyridine	242
S	
styrene	144
T	
n-tetradecane	43
1-tetradecene	82
tetrahydrofuran	256
toluene	133
n-tridecane	42
1-tridecene	81
triethyl amine	245
trimethyl amine	238
U	
n-undecane	40
1-undecene	79
V	
valeric acid	205
vinyl acetate	222
vinyl chloride	150
vinyl fluoride *	163
X	
o-xylene	135
m-xylene	136
p-xylene	137

Using an Optional Printer with the Programs

If you run a chemical engineering program when a printer is connected to the calculator, the program automatically gives you a printed record of all calculations. (For information on setting up a printer, refer to "Printer Device Numbers" and "Setting the Printer Format" in Chapter 6 of the *TI-95 User's Guide*.)

Advantages of Using a Printer

A printer gives you a convenient method of reviewing the results of your calculations. The printout includes:

- The name of the program.
- The data values you entered. (This also enables you to see if you entered the values correctly.)
- Any options you selected.
- The results of the calculations, along with labels that identify each result.

Without a printer, you need to press a key to display each result. With a printer, the program does not stop to display individual results. Instead, the program prints a continuous list of results until the output is complete.

When to Connect a Printer

When you select a program, the calculator immediately checks to see if a printer is connected.

- If you want a printout, connect the printer before selecting the program.
- If you do not want a printout, disconnect the printer before selecting the program.

Precaution When Using a Printer

When you are using a printer with a cartridge program, be sure the calculator is not in the Trace mode (exit the Trace mode by pressing [INV] [2nd] [TRACE]). In the Trace mode, the calculator prints each program step as it is executed. This slows the operation of the program and uses a large amount of paper.

Even when no printer is connected, you should avoid running a cartridge program in the Trace mode because the calculator pauses after each program step.

Chapter 2: Properties Table

This chapter assists you in using the Properties Table program, which recalls several intrinsic properties for many industrial organic compounds.

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The Properties Table Program

The Properties Table program provides you with the properties of a compound. The values in this built-in table are accessed by many of the programs in the Chemical Engineering library.

Selecting the Program

To select the Properties Table program:

1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:

2. Select ⟨TAB⟩. The program displays:

Enter the number of a compound and press ⟨#⟩ to specify the compound.

Obtaining the Results

After you specify the compound, the program displays:

The number displayed before you make a selection is the last value generated (Mw).

⟨tc⟩ Displays the critical temperature in °C.

⟨Pc⟩ Displays the critical pressure in atmospheres.

⟨Vc⟩ Displays the critical specific volume in cm^3/g-mole.

⟨tb⟩ Displays the boiling temperature in °C for a pressure of 1 atmosphere.

⟨-->⟩ Displays the next group of menu selections (shown on the next page).

The number displayed before you make a selection is left over from the previous menu.

⟨w⟩ Displays the acentric factor.

⟨CpA⟩ Displays the A gas specific heat coefficient.

⟨CpB⟩ Displays the B gas specific heat coefficient.

⟨CpC⟩ Displays the C gas specific heat coefficient.

⟨-->⟩ Displays the next group of menu selections (shown below).

The number displayed before you make a selection is left over from the previous menu.

⟨Cpn⟩ Displays the n gas specific heat coefficient (hydrocarbons only).

⟨CpD⟩ Displays the D gas specific heat coefficient.

⟨Zra⟩ Displays the Rackett parameter for saturated liquid density estimation.

⟨Mw⟩ Displays the molecular weight.

⟨-->⟩ Displays the first group of menu selections (shown on the previous page).

View each property that you want to see by pressing the key that corresponds to that property.

Example: Obtaining the Properties of a Compound

The following example illustrates how to use the Properties Table program.

Example

Determine the properties of benzene, which is compound number 132 in the list of compounds.

Procedure	Press		Display
Select program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨TAB⟩		PROPERTIES TABLE
Enter benzene	132 ⟨#⟩		78.114
Display the properties	⟨tc⟩	tc =	288.95
	⟨Pc⟩	Pc =	48.3
	⟨Vc⟩	Vc =	259.
	⟨tb⟩	tb =	80.15
	⟨-->⟩ ⟨w⟩	w =	0.212
	⟨CpA⟩	CpA =	8.5813
	⟨CpB⟩	CpB =	65.2801
	⟨CpC⟩	CpC =	1167.4835
	⟨-->⟩ ⟨Cpn⟩	Cpn =	1.1377
	⟨CpD⟩	CpD =	0.
	⟨Zra⟩	Zra =	0.26967
	⟨Mw⟩	Mw =	78.114

Chapter 3: Gas Properties

This chapter describes how to use the Gas Viscosity Property program and the Gas Thermal Conductivity Property program.

Table of Contents

Gas Viscosity Introduction

The Gas Viscosity Property program estimates the viscosity of nonpolar and polar gases at different pressures. In addition, the program treats hydrogen-bonding and non-hydrogen-bonding polar gases separately.

Method of Estimation—Low Pressure

This program uses the corresponding-states method developed by Thodos[1] to estimate vapor viscosities at low pressures. The method has its origin in the hard-sphere kinetic theory of gases. The program requires that you classify the vapor as either a polar or nonpolar gas.

Nonpolar Gases

For nonpolar gases, the empirical equation for low pressure viscosity is

$$\mu\xi = 4.61T_r^{0.618} - 2.04e^{-0.449T_r} + 1.94e^{-4.058T_r} + .1$$

where

$$\xi = T_c^{1/6} M_W^{-1/2} P_c^{-2/3}$$

Polar Gases

Polar gases are divided further into hydrogen-bonding types, which are represented by the equation

$$\mu\xi = (0.755T_r - 0.055)Z_c^{-5/4} \qquad T_r < 2.0$$

and non-hydrogen-bonding types, which are correlated using the expression

$$\mu\xi = (1.90T_r - 0.29)^{4/5} Z_c^{-2/3}$$

Pressure

Pressure has a significant effect on the viscosity of a gas or vapor. The most accurate way to account for the effect of pressure is through residual viscosity-density correlations. For nonpolar gases[2], the pressure effect is given by

$$[(\mu-\mu^0)\xi+1]^{0.25}=1.023+0.23364\rho_r+0.58533\rho_r^2-0.40758\rho_r^3+0.093324\rho_r^4 \qquad .1\leq\rho_r\leq 3$$

The form of correlation for polar gases[3] depends upon the reduced density, as seen in the equations below.

$$(\mu-\mu^0)\xi=1.656\rho_r^{1.111} \qquad \rho_r\leq 0.1$$

$$(\mu-\mu^0)\xi=0.0607(9.045\rho_r+0.63)^{1.739} \qquad 0.1<\rho_r\leq 0.9$$

$$\log[4-\log[(\mu-\mu^0)\xi]]=0.6439-0.1005\rho_r-\Delta \qquad 0.9<\rho_r<2.6$$

where

$$\Delta=\begin{cases}0 & 0.9<\rho_r\leq 2.2\\ (4.75)(10^{-4})(\rho_r^3-10.65)^2 & 2.2<\rho_r<2.6\end{cases}$$

The high pressure option should be used any time the pressure is more than ten atmospheres.

Mixtures

The program employs the method of Dean and Stiel[4] for calculating the viscosity of a gas mixture. Low pressure mixture viscosity is given by:

$$\eta_m\xi_m=\begin{cases}3.4T_{r_m}^{8/9} & T_{r_m}\leq 1.5\\ 16.68(0.1338T_{r_m}-0.0932)^{5/9} & T_{r_m}>1.5\end{cases}$$

where $\xi_m=\dfrac{T_{c_m}^{1/6}}{P_{c_m}^{2/3}(\sum_i y_iM_i)^{1/2}}$

$$T_{r_m}=T/T_{c_m} \qquad T_{c_m}=\sum_i y_iT_{c_i}$$

$$Z_{c_m}=\sum_i y_iZ_{c_i} \qquad V_{c_m}=\sum_i y_iV_{c_i}$$

$$P_{c_m}=\frac{Z_{c_m}RT_{c_m}}{V_{c_m}}$$

η_m = low pressure viscosity, μP

Mixtures (Continued)

The residual viscosity correlation of Dean and Stiel calculates the high pressure viscosity based on the low pressure viscosity.

$$(\eta_m - \eta_m^\circ)\xi_m = (1.08)\,[\exp(1.439\rho_{r_m}) - \exp(-1.11\rho_{r_m}^{1.858})]$$

where η_m = high pressure mixture viscosity, μP

η_m° = low pressure mixture viscosity, μP

ρ_{r_m} = pseudoreduced mixture density, $\rho_m v_{c_m}$

ρ_m = mixture density, g mole/cm^3

$$\xi_m = T_{c_m}^{1/6} / (M_m^{1/2} P_{c_m}^{2/3})$$

$$M_m = \sum_i y_i M_i$$

$$\eta_m = \frac{f(\rho_{r_m}) + \eta_m^\circ \xi_m}{\xi_m}$$

References

1 Yoon, P., and Thodos, G. 1970. Viscosity of Nonpolar Gaseous Mixtures at Normal Pressures. *AIChE Journal* 2: 300.

2 Jossi, J. A.; Stiel, L. I.; and Thodos, G. 1962. The Viscosity of Pure Substances in the Dense Gaseous and Liquid Phases. *AIChE Journal* 1: 59.

3 Stiel, L. I., and Thodos, G. 1964. The Viscosity of Polar Substances in the Dense Gaseous and Liquid Regions. *AIChE Journal* 2: 275.

4 Dean, D. E., and Stiel, L. I. 1965. The Viscosity of Nonpolar Gas Mixtures at Moderate and High Pressures. *AIChE Journal* 11: 526.

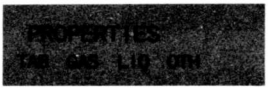
The Gas Viscosity Property Program

The following procedure provides instructions for using the Gas Viscosity Property program.

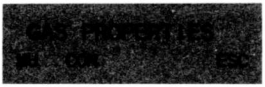
Selecting the Program

To select the Gas Viscosity Property program:

1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:



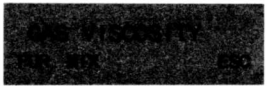
2. Select ⟨GAS⟩. The program displays:



3. Select ⟨MU⟩.

Selecting an Option

After you select the program, the following display appears.



- To calculate the viscosity of a pure gas, press ⟨PUR⟩. The instructions for this option begin on the next page.
- To calculate the viscosity of a gas mixture, press ⟨MIX⟩. Go to page 3–10 for the instructions for this option.

The Pure Gas Viscosity Option

The following procedure provides instructions for using the pure gas viscosity option of the Gas Viscosity program.

Specifying a Compound and Its Conditions

After you select the pure gas viscosity option, the program displays:

You can check the current entries by pressing [INV] ⟨#⟩ or [INV] ⟨t⟩. To specify the compound and its conditions:

1. Enter the number of the compound and press ⟨#⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."

2. Enter the system temperature in °C and press ⟨t⟩.

3. Decide whether to use the high pressure gas viscosity model or the low pressure gas viscosity model.

   - If the high pressure model applies, press ⟨HIp⟩ to proceed with the program.

   - If the low pressure model applies, press ⟨LOp⟩ to proceed with the program.

Specifying the Properties

After you specify the compound and its conditions, the program displays a menu of the properties.

The number displayed before you make a selection is the last value generated (Mw).

Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the values for tc, Pc, Vc, and Mw without checking them.

You can check the current entries by pressing INV ⟨tc⟩, INV ⟨Pc⟩, INV ⟨Vc⟩, or INV ⟨Mw⟩. To enter the properties:

1. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.

2. If you want to change the value for the critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.

3. If you want to change the value for the critical specific volume, enter the new value in cm^3/g-mole and press ⟨Vc⟩.

4. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.

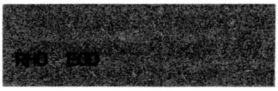
5. If you enter an incorrect value, enter the correct value and press the corresponding key.

6. Press ⟨EOD⟩ to proceed with the program.

Specifying the Properties (Continued)

The display that appears next depends on the pressure model you selected.

- If you selected the low pressure model, proceed to the **POLAR?** menu below.
- If you selected the high pressure model, the program prompts you to enter the density.

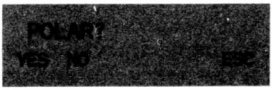


The number displayed when this menu first appears is left over from the previous menu.

You can check the current entry for density by pressing INV ⟨RHO⟩. To enter a value for density:

1. Determine the density in gram moles per cm^3.
2. Enter the value and press ⟨RHO⟩.
3. If you enter an incorrect value, enter the correct value and press ⟨RHO⟩.
4. Press ⟨EOD⟩ to proceed with the program.

The program then prompts you to indicate whether the molecule is polar.

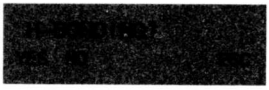


- If the molecule is polar, press ⟨YES⟩ and go to the top of the next page.
- If the molecule is nonpolar, press ⟨NO⟩ and go to "Obtaining the Result" on the next page.

(continued)

Specifying the Properties (Continued)

The program then prompts you to indicate whether the molecule is hydrogen bonding.



- If the molecule is hydrogen bonding, press ⟨YES⟩ and proceed with the result.
- If the molecule is not hydrogen bonding, press ⟨NO⟩ and proceed with the result.

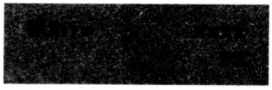
Obtaining the Result

After you have specified the properties, the display that appears depends on the pressure model you selected.

- If you selected the low pressure model, the program displays:

where xxxx is the gas viscosity in micropoise.

- If you selected the high pressure model, the program displays:



where xxxx is the gas viscosity in micropoise.

The Gas Mixture Viscosity Option

The following procedure provides instructions for using the gas mixture viscosity option of the Gas Viscosity program.

Defining the Mixture

After you select the option for viscosity of a gas mixture, the program displays:

You can check the current entries by pressing [INV] ⟨n⟩ or [INV] ⟨t⟩. To define the mixture:

1. Enter the number of compounds in the mixture and press ⟨n⟩.
2. Enter the system temperature in °C and press ⟨t⟩.
3. Decide whether to use the high pressure gas viscosity model or the low pressure gas viscosity model.
   - ► If the high pressure model applies, press ⟨Hlp⟩ to proceed with the program.
   - ► If the low pressure model applies, press ⟨LOp⟩ to proceed with the program.

Entering a Component Gas

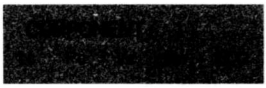
After you define the mixture, the program displays:

To specify a component gas:

1. Enter the number of the compound for this component and press ⟨ENT⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."
2. Press ⟨EOD⟩ to proceed with the program.

Entering the Properties

After you enter the first component, the program displays:



Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the values for tc, Pc, Vc, and Mw without checking them.

You can check the current entries by pressing [INV] ⟨tc⟩, [INV] ⟨Pc⟩, [INV] ⟨Vc⟩, or [INV] ⟨Mw⟩. To enter the properties:

1. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.

2. If you want to change the value for the critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.

3. If you want to change the value for the critical specific volume, enter the new value in cm^3/g-mole and press ⟨Vc⟩.

4. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.

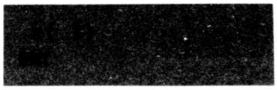
5. If you enter an incorrect value, enter the correct value and press the corresponding key.

6. Press ⟨EOD⟩ to proceed with the program.

The program repeats the entry sequence for each component.

Entering the Mole Fractions

After you enter the properties of the last component, the program prompts you to enter the mole fraction for each component except the last.



You can check the current entry by pressing CE. To enter a mole fraction:

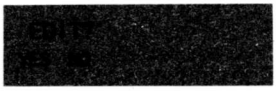
1. Enter a value for the mole fraction of this component and press ⟨ENT⟩.

2. Repeat step 1 for each component except the last.

Because the total of all the mole fractions of a mixture must be one, the program determines the last mole fraction without your entering it.

Editing the Mole Fractions

After the program determines the last mole fraction, it displays:



- If you want to edit a value, press ⟨YES⟩ and return to the top of this page.

- If you do not want to edit any values, press ⟨NO⟩.

Obtaining the Result

After you have specified the properties, the display that appears depends on the pressure model you selected.

- If you selected the low pressure model, the program displays:

where xxxx is the gas viscosity in micropoise.

- If you selected the high pressure model, the program displays:

where xxxx is the gas viscosity in micropoise.

Example 1: Estimating Viscosity of a Pure Gas

The following example illustrates how to use the Gas Viscosity Property program to estimate the viscosity of a pure gas.

Example

Estimate the viscosity of n-pentane (compound 6) vapor at 100 °C and 1 atmosphere of pressure. This molecule is nonpolar.

Procedure	Press	Display	
Select program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨GAS⟩ ⟨MU⟩ ⟨PUR⟩	PURE GAS VISCOS	
Enter the compound and its conditions	6 ⟨#⟩ 100 ⟨t⟩ ⟨LOp⟩		72.151
Accept the properties generated by the program	⟨EOD⟩	POLAR?	
View the gas viscosity	⟨NO⟩	MUlo =	87.

Note: The literature value for the vapor viscosity of n-pentane at 100 °C is 88 micropoise. The estimated value has an error of 1.14%. For the compounds tested with this program, the average error was 1.33% at low pressure and −14.43% at high pressure.

Example 2: Estimating Viscosity of a Gas Mixture

The following example illustrates how to use the Gas Viscosity Property program to estimate the viscosity of a gas mixture.

Example

A mixture at 100 °C and 1 atmosphere consists of two compounds: acetone (compound 211) and n-pentane (compound 6).

Estimate the viscosity if a 0.1 mole fraction of the mixture is the first compound and the rest of the mixture is the second compound.

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨GAS⟩ ⟨MU⟩ ⟨MIX⟩	GAS MIX VISCOS
Define the mixture	2 ⟨n⟩ 100 ⟨t⟩ ⟨LOp⟩	#(1)
Enter the compound	211 ⟨ENT⟩ ⟨EOD⟩	COMPONENT(1)
Accept the properties generated by the program	⟨EOD⟩	#(2)
Enter the compound	6 ⟨ENT⟩ ⟨EOD⟩	COMPONENT(2)
Accept the properties generated by the program	⟨EOD⟩	x(1)
Enter the mole fraction of the first component	.1 ⟨ENT⟩	EDIT?
View the gas viscosity	⟨NO⟩	MUlo = 87.

Gas Thermal Conductivity Introduction

This section describes the Gas Thermal Conductivity Property program, which estimates the thermal conductivity of pure gases at low and high pressures (Misic-Thodos and Stiel-Thodos methods) and of mixtures (Wassiljewa-Lindsay-Bromley correlation).

Method of Estimation—Low Pressure

For low pressures, the program uses the method of Misic and Thodos[1,2]. The Misic and Thodos expression

$$\lambda_o = (10^{-6})(14.52T_r - 5.14)^{2/3}C_p/\Gamma$$

$$\text{where } \Gamma = \frac{T_c^{1/6}M_w^{1/2}}{P_c^{2/3}}$$

has its origin in a dimensional analysis approach.

Method of Estimation—High Pressure

For higher pressures, the program uses the Stiel and Thodos[3] correlations to estimate the thermal conductivity:

$$\lambda = \lambda_o + (14.0\times10^{-8})(e^{0.535\rho_r} - 1)/\Gamma Z_c^5 \qquad \rho_r \leq 0.5$$

$$\lambda = \lambda_o + (13.1\times10^{-8})(e^{0.67\rho_r} - 1.069)/\Gamma Z_c^5 \qquad 0.5 < \rho_r \leq 2.0$$

$$\lambda = \lambda_o + (2.976\times10^{-8})(e^{1.155\rho_r} + 2.016)/\Gamma Z_c^5 \qquad 2.0 < \rho_r < 2.8$$

Note that the low-pressure thermal conductivity is part of the estimation technique. The Stiel and Thodos method is limited to $\rho_r < 2.8$.

Method of Estimation—Mixtures

For mixtures, the program uses pure component thermal conductivities in the Wassiljewa-Lindsay-Bromley[4] correlation to estimate a mixture's thermal conductivity. This correlation uses the empirical parameter

$$A_{ij} = \frac{1}{4}\left[1 + \left[\frac{n_i}{n_j}\left(\frac{m_j}{m_i}\right)^{3/4}\frac{T+S_i}{T+S_j}\right]^{1/2}\right]^2\frac{T+S_{ij}}{T+S_i}$$

$$\text{where } S_i = 1.5T_{bi} \qquad S_j = 1.5T_{bj} \qquad S_{ij} = (S_iS_j)^{1/2}$$

Then, to calculate a mixture's thermal conductivity, the program uses

$$\lambda_{mix} = \sum_{i=1}^{n}\frac{y_i\lambda_i}{\sum_{j=1}^{n} y_i\lambda_j}$$

References

[1] Misic, D., and Thodos, G. 1961. The Thermal Conductivity of Hydrocarbon Gases at Normal Pressures. *AIChE Journal* 2: 264.

[2] Misic, D., and Thodos, G. 1963. Atmospheric Thermal Conductivities for Gases of Simple Molecular Structure. *Journal of Chemical and Engineering Data* 4: 540.

[3] Stiel, L. I., and Thodos, G. 1964. The Thermal Conductivity of Nonpolar Substances in the Dense Gaseous and Liquid Regions. *AIChE Journal* 1: 26.

[4] Lindsay, A. L., and Bromley, L. A. 1950. Thermal Conductivity of Gas Mixtures. *Industrial and Engineering Chemistry* 8: 1508.

The Gas Thermal Conductivity Property Program

The following procedure provides instructions for using the Gas Thermal Conductivity Property program.

Before You Select the Program

Before you select this program, you need values for specific heat and possibly viscosity.

- If you do not have the value for specific heat, obtain it from the specific heat program (page 6-21) before selecting this program.
- If you are analyzing a gas mixture and do not have the values for viscosity, obtain them from the gas viscosity program (page 3-2) before selecting this program.

Selecting the Program

To select the Gas Thermal Conductivity program:

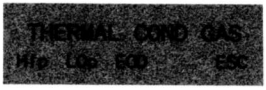
1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:

2. Select ⟨GAS⟩. The program displays:

3. Select ⟨CON⟩.

Selecting a Pressure Option

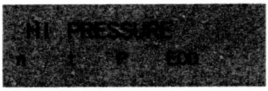
After you select the program, the following display appears.



- If the high pressure gas model applies, press ⟨HIp⟩ ⟨EOD⟩. Then proceed with "Defining a High-Pressure Mixture" on the next page.
- If the low pressure gas model applies, press ⟨LOp⟩ ⟨EOD⟩. Then proceed with "Defining a Low-Pressure Mixture" on page 3-23.

Defining a High-Pressure Mixture

If you select the high pressure option, the program displays the following menu.

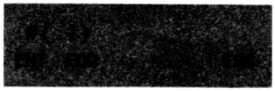


You can check the current entries by pressing INV ⟨n⟩, INV ⟨t⟩, or INV ⟨P⟩. To define the mixture:

1. Enter the number of components and press ⟨n⟩. A mixture of only one component is a pure substance.
2. Enter the system temperature in °C and press ⟨t⟩.
3. Enter the system pressure in atmospheres and press ⟨P⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Specifying a Component Gas

After you define the mixture, the program displays:



You can check the current entry by pressing CE. To specify a component gas:

1. Enter the number of the compound for this component and press ⟨ENT⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."
2. Press ⟨EOD⟩ to proceed with the program.

Entering the Properties

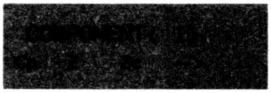
After you specify the first component, the program displays:

Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You must supply values for Cp, Z, Zc, and MU. You can generally accept the values for tc, Pc, Mw and tb without checking them.

You can check the current entries by pressing INV ⟨tc⟩, INV ⟨Pc⟩, or INV ⟨Mw⟩. To enter the properties:

1. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.
2. If you want to change the value for the critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.
3. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.
4. Press ⟨-->⟩ to display additional selections shown on the next page.

Entering the Properties (Continued)



You can check the current entries by pressing [INV] ⟨Cp⟩, [INV] ⟨Z⟩, or [INV] ⟨Zc⟩. To continue entering the properties:

5. Enter a value for the specific heat in calories per gram-°C and press ⟨Cp⟩.

6. If you want to change the value for the compressibility factor, enter the new value and press ⟨Z⟩.

7. Enter a value for the critical compressibility factor and press ⟨Zc⟩.

8. What you should do next depends on the number of components you specified.

   ► If you specified 1 component, the menu includes ⟨EOD⟩.

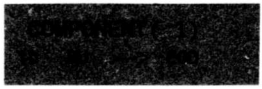
   If you want to review the previous selections shown on the preceding page, press ⟨-->⟩. If you enter an incorrect value, enter the correct value and press the corresponding key. Then press ⟨EOD⟩ to proceed with the program. Go to page 3–27.

   ► If you specified a mixture of components, the menu has no ⟨EOD⟩.

   Press ⟨-->⟩ to display additional selections shown on the next page.

(continued)

Entering the Properties (Continued)



You can check the current entries by pressing [INV] ⟨tb⟩ or [INV] ⟨MU⟩. To continue entering the properties:

9. If you want to change the value for the boiling temperature, enter the new value in °C and press ⟨tb⟩.

10. Enter a value for the component viscosity in micropoise and press ⟨MU⟩.

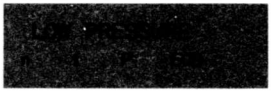
11. If you want to review the previous selections shown on page 3-20, press ⟨-->⟩.

12. Press ⟨EOD⟩ to proceed with the program.

The program repeats the entry sequence for each component. After you enter the properties of the last component, go to page 3-26.

Defining a Low-Pressure Mixture

If you select the low pressure option, the program displays the following menu.

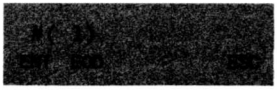


You can check the current entries by pressing INV ⟨n⟩, INV ⟨t⟩, or INV ⟨P⟩. To define the mixture:

1. Enter the number of components and press ⟨n⟩.
2. Enter the system temperature in °C and press ⟨t⟩.
3. Enter the system pressure in atmospheres and press ⟨P⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Specifying a Component Gas

After you define the mixture, the program displays:



To specify a component gas:

1. Enter the number of the compound for this component and press ⟨ENT⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."
2. Press ⟨EOD⟩ to proceed with the program.

Entering the Properties

After you specify the first component, the program displays:

Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You must supply values for Cp, Z, Zc, and MU. You can generally accept the values for tc, Pc, Mw and tb without checking them.

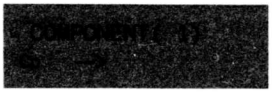
You can check the current entries by pressing INV ⟨tc⟩, INV ⟨Pc⟩, or INV ⟨Mw⟩. To enter the properties:

1. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.

2. If you want to change the value for the critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.

3. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.

4. Press ⟨-->⟩ to display additional selections shown below.



You can check the current entry by pressing INV ⟨Cp⟩. To continue entering the properties:

5. Enter a value for the specific heat in calories per gram-°C and press ⟨Cp⟩.

Entering the Properties (Continued)

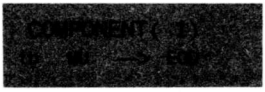
6. What you should do next depends on the number of components you specified.

   - If you specified 1 component, the menu includes ⟨EOD⟩.

     If you want to review the previous selections shown on the preceding page, press ⟨-->⟩. If you enter an incorrect value, enter the correct value and press the corresponding key. Then press ⟨EOD⟩ to proceed with the program. Go to page 3-27.

   - If you specified a mixture of components, the menu has no ⟨EOD⟩.

     Press ⟨-->⟩ to display additional selections shown below.



You can check the current entries by pressing INV ⟨tb⟩ or INV ⟨MU⟩. To continue entering the properties:

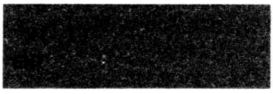
7. If you want to change the value for the boiling temperature, enter the new value in °C and press ⟨tb⟩.
8. Enter a value for the component viscosity in micropoise and press ⟨MU⟩.
9. If you want to review the previous selections shown on the preceeding page, press ⟨-->⟩.
10. Press ⟨EOD⟩ to proceed with the program.

The program repeats the entry sequence for each component. After you enter the properties of the last component, proceed to the next page.

Entering the Mole Fractions

The display that appears next depends on the number of components in the mixture.

- If the mixture contains only one component, the result is displayed, as shown on the next page.
- If the mixture contains more than one component, the program displays:



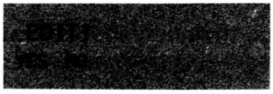
You can check the current entry by pressing CE. To enter a mole fraction:

1. Enter a value for the mole fraction of this component and press ⟨ENT⟩.
2. Repeat step 1 for each component except the last.

   Because the total of all the mole fractions of a mixture must be one, the program determines the last mole fraction without your entering it.

Editing the Mole Fractions

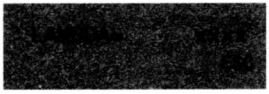
After the program determines the last mole fraction, it displays an **EDIT?** menu that allows you to change any of the mole fraction entries.



- If you want to edit a value, press ⟨YES⟩ and go to "Entering the Mole Fractions" on this page.
- If you do not want to edit any values, press ⟨NO⟩.

Obtaining the Result

After you select not to edit, the program displays the result.



where xxxx is the thermal conductivity expressed in calories per cm-second-°C.

Example: Estimating Gas Thermal Conductivity

The following example illustrates how to use the Gas Thermal Conductivity Property program.

Example

Find the thermal conductivity of n-pentane (compound 6) at 100 °C and 1 atmosphere.

Cp = 0.478 cal/g-°C

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨GAS⟩ ⟨CON⟩	THERMAL COND GAS
Define the mixture	⟨LOp⟩ ⟨EOD⟩ 1 ⟨n⟩ 100 ⟨t⟩ 1 ⟨P⟩ ⟨EOD⟩	#(1)
Enter the compound	6 ⟨ENT⟩ ⟨EOD⟩	COMPONENT(1)
Enter the missing property	⟨-->⟩ .478 ⟨Cp⟩ ⟨EOD⟩	LAMBDA = 0.000052

The thermal conductivity is 0.000052 calories per centimeter-second-°C.

Note: The literature value of the vapor thermal conductivity of n-pentane at 100 °C is 0.000056 cal/cm-sec-°C. The program's estimated value has an error of −7.14%. For the compounds tested with this program, the average error was −1.19%.

Chapter 4: Liquid Properties

This chapter describes how to use the Liquid Viscosity Property program, the Liquid Thermal Conductivity Property program, and the Liquid Density Property program.

Table of Contents

Liquid Viscosity Introduction

The Liquid Viscosity Property program estimates liquid viscosity for hydrocarbons and nonhydrocarbons at various temperatures. It also estimates viscosity for binary mixtures at moderate temperatures.

Method of Estimation—Hydrocarbons, Low Temperatures

For hydrocarbons, this program uses the generalized expression developed by Thomas[1] to estimate liquid-phase viscosity for hydrocarbons. The correlation is valid only for $T_r < 0.7$. In the expression

$$\log(8.569\mu_L/\rho_L^{1/2}) = \theta(1/T_r - 1)$$

θ is a viscosity parameter that depends on the molecular structure of the compound. Refer to "Tables for Liquid Viscosity" in this chapter when you determine group contributions. The liquid density at the temperature of interest is ρ_L.

Method of Estimation—Nonhydrocarbons, Low Temperatures

For nonhydrocarbons, the program uses the correlation developed by Orrick and Erbar[2]. In the expression

$$\ln(\mu_L/\rho_L M_W) = A + B/T$$

where

$$A = (.695 + 0.21n) + GC(A)$$
$$B = 275 + 99n + GC(B)$$

GC(A) and GC(B) are the group contributions developed from values in the "Tables for Liquid Viscosity" section, and n is the number of carbon atoms not included in the group contributions.

Method of Estimation—High Temperatures

For higher temperatures, the program uses the formula of Letsou and Stiel[3]. The expression

$$\mu_L\xi = (\mu_L\xi)^0 + \omega(\mu_L\xi)^1$$

where

$$(\mu_L\xi)^0 = 0.015174 - 0.02135T_r + 0.0075T_r^2$$
$$(\mu_L\xi)^1 = 0.042552 - 0.07674T_r + 0.034T_r^2$$

and

$$\xi = T_c^{1/6}/(M_w^{1/2}P_c^{2/3})$$

is based on the corresponding-states approach to fluid behavior. The Letsou-Stiel equation is used in the temperature range $0.7 < T_r < 0.98$.

Binary Mixtures—Moderate Temperatures

The program estimates viscosity for binary mixtures through the formula proposed by Lobe[4].

$$\nu_m = \phi_1\nu_1 e^{\phi_2\alpha_2} + \phi_2\nu_2 e^{\phi_1\alpha_1}$$

where

$$\alpha_1 = -1.7\ln(\nu_2/\nu_1)$$

$$\alpha_2 = 0.27\ln(\nu_2/\nu_1) + [1.3\ln(\nu_2/\nu_1)]^{1/2}$$

and

$$\phi_1 = x_1\nu_{L1}/(x_1\nu_{L1} + x_2\nu_{L2})$$
$$\phi_2 = x_2\nu_{L2}/(x_1\nu_{L1} + x_2\nu_{L2})$$
$$\nu = \mu/\rho$$

Here x_1 and x_2 are the mole fractions of components 1 and 2, respectively. This expression is good only at moderate temperatures.

References

[1] Thomas, L. H. 1946. The Dependence of the Viscosities of Liquids on Reduced Temperature and a Relation of Viscosity, Density, and Chemical Constitution. *Journal of the Chemical Society* p. 573.

[2] Reid, R. C.; Prausnitz, J. M.; and Sherwood,T. K. 1977. *Properties of Gases and Liquids.* 3rd ed. (citing Orrick, C., and Erbar, J. H.). New York: McGraw-Hill.

[3] Letsou, A., and Stiel, L. I. 1973. Viscosity of Saturated Nonpolar Liquids at Elevated Pressures. *AIChE Journal* 2: 409.

[4] Lobe, V. M. 1973. M. S. Thesis, University of Rochester, Rochester, N. Y.

The following procedure provides instructions for using the Liquid Viscosity Property program.

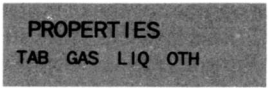
Before You Select the Program

If you are analyzing a liquid for which the hydrocarbon specific heat model applies and you do not have the value for density, obtain it from the Liquid Density Property program (page 4-26) before selecting this program.

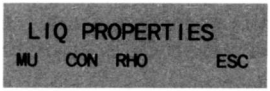
Selecting the Program

To select the Liquid Viscosity Property program:

1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:



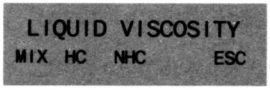
2. Select ⟨LIQ⟩. The program displays:



3. Select ⟨MU⟩.

Selecting an Option

After you select the program, the following display appears.

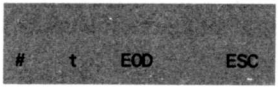


- If you are calculating the viscosity of a binary mixture, press ⟨MIX⟩ to select the binary mixture option and turn to page 4-14.
- If you are calculating the viscosity of a pure liquid from the Thomas Correlation or the Letsou and Stiel Correlation, press ⟨HC⟩ to select the hydrocarbon option and turn to the next page.
- If you are calculating the viscosity of a pure liquid from the Orrick and Erbar Correlation or the Letsou and Stiel Correlation, press ⟨NHC⟩ to select the nonhydrocarbon option and turn to the next page.

The following procedure provides instructions for using the pure liquid options of the Liquid Viscosity Property program.

Specifying a Compound and Its Temperature

If you select an option for a pure liquid, the program displays:



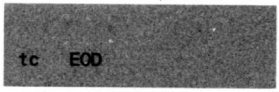
The message displayed is the option selected from the previous menu.

You can check the current entries by pressing INV ⟨#⟩ or INV ⟨t⟩. To specify a compound and its temperature:

1. Enter the number of the compound and press ⟨#⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."
2. Enter a value for the temperature in °C and press ⟨t⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.

Entering the Critical Temperature

After you specify the compound and its temperature, the program displays:



The number displayed is the last value generated (tc).

You can check the current entry by pressing INV ⟨tc⟩. If this value is satisfactory, press ⟨EOD⟩ to proceed with the program. To enter the critical temperature:

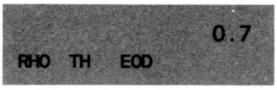
1. Enter a value for the critical temperature in °C and press ⟨tc⟩.
2. If you enter an incorrect value, enter the correct value and press ⟨tc⟩.
3. Press ⟨EOD⟩ to proceed with the program.

After you accept or enter the critical temperature, the program calculates the temperature ratio, which partially determines the calculation method.

- If the temperature ratio is less than .7 and you selected ⟨HC⟩ earlier, the program uses the Thomas (hydrocarbon) correlation. Go to the next page.
- If the temperature ratio is less than .7 and you selected ⟨NHC⟩ earlier, the program uses the Orrick and Erbar (nonhydrocarbon) correlation. Go to page 4–9.
- If the temperature ratio is between .7 and .98, the program uses the Letsou and Stiel correlation regardless of your earlier selection of ⟨HC⟩ or ⟨NHC⟩. Go to page 4–11.
- If the temperature ratio is greater than 0.98, the program displays **Tr>.98**. Press ⟨ESC⟩ to repeat the input sequence so you can enter different temperature values. Go to "Selecting an Option" on page 4–5.

Entering Data for Hydrocarbon Viscosity

If the compound is a hydrocarbon and the temperature ratio is less than 0.7, the following display appears.



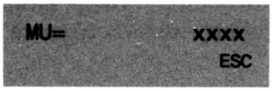
The number displayed is to be ignored.

You can check the current entries by pressing [INV] ⟨RHO⟩ or [INV] ⟨TH⟩. To enter the data for hydrocarbon viscosity:

1. Enter the value for density in grams per cm^3 and press ⟨RHO⟩.
2. Determine the total of structural contributions from the table on page 4-12.
3. Enter the value for total structural contributions and press ⟨TH⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Obtaining the Hydrocarbon Result

After you enter the data for hydrocarbon viscosity, the following display appears.



where xxxx is the value for viscosity in centipoise.

Entering Data for Nonhydrocarbon Viscosity

If the program determines the temperature ratio to be less than 0.7, the following display appears.

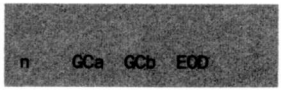
The number displayed is the last value generated (Mw).

You can check the current entries by pressing [INV] ⟨RHO⟩ or [INV] ⟨Mw⟩. To enter the data needed to calculate the nonhydrocarbon viscosity:

1. Enter the value for density in grams per cm^3 and press ⟨RHO⟩.
2. Enter the value for molecular weight and press ⟨Mw⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.

Entering the Group Contributions

After you enter the data for nonhydrocarbon viscosity, the program displays:



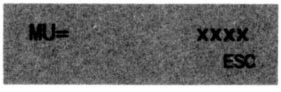
The number displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨n⟩, INV ⟨GCa⟩, or INV ⟨GCb⟩. To enter the group contributions:

1. Define your molecule in terms of the groups listed in the table on page 4–12.
2. Count the carbon atoms that are not in a group contribution. Enter this value and press ⟨n⟩.
3. Add the A values for all group contributions in your molecule. Enter this value and press ⟨GCa⟩.
4. Add the B values for all group contributions in your molecule. Enter this value and press ⟨GCb⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ to proceed with the program.

Obtaining the Nonhydrocarbon Result

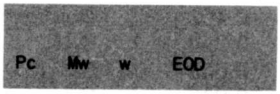
After you enter the group contributions, the following display appears.



where xxxx is the value for viscosity in centipoise.

Entering Data for Viscosity at Higher Reduced Temperatures

If the reduced temperature is greater than or equal to 0.7, but less than or equal to 0.98, the program displays:



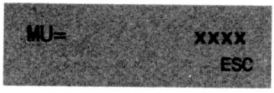
The number displayed is the last value generated (Mw).

You can check the current entries by pressing INV ⟨Pc⟩, INV ⟨Mw⟩, or INV ⟨w⟩. To enter the data needed to calculate the hydrocarbon viscosity:

1. Enter the value for critical pressure in atmospheres and press ⟨Pc⟩.
2. Enter the value for molecular weight and press ⟨Mw⟩.
3. Enter the value for the acentric factor and press ⟨w⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Obtaining the Viscosity at Higher Reduced Temperatures

After you enter the data for a reduced temperature greater than 0.7, the following display appears.



where xxxx is the value for viscosity in centipoise.

Table of Structural Contributions (Thomas Method)

Structural Component	Contribution	Structural Component	Contribution
C	−0.462	Double bond	0.478
H	0.249	C_6H_5	0.385
O	0.054	S	0.043
Cl	0.340	CO (ketones)	0.105
Br	0.326	CO (esters)	0.105
I	0.335	CN (nitrile)	0.381

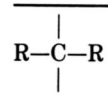
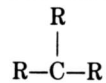
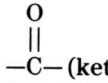
Structural Contributions Source

Thomas, L. H. 1946. The Dependence of the Viscosities of Liquid on Reduced Temperature and a Relation of Viscosity, Density, and Chemical Constitution. *Journal of the Chemical Society* p. 573.

Group Contributions Source

Reid, R. C.; Prausnitz, J. M.; and Sherwood,T. K. 1977. *Properties of Gases and Liquids*. 3rd ed. (citing Orrick, C., and Erbar, J. H.). New York: McGraw-Hill.

Table of Group Contributions (Orrick and Erbar Method)

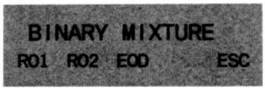
Group	A	B
	−0.15	35
	−1.20	400
Double bond	0.24	−90
Five-membered ring	0.10	32
Six-membered ring	−0.45	250
Aromatic ring	0	20
Ortho substitution	−0.12	100
Meta substitution	0.05	−34
Para substitution	−0.01	−5
Chlorine	−0.61	220
Bromine	−1.25	365
Iodine	−1.75	400
—OH (alcohol)	−3.00	1600
—COO— (ester)	−1.00	420
—O— (ether)	−0.38	140
	−0.50	350
—COOH (acid)	−0.90	770

The Binary Mixture Option

The following procedure provides instructions for using the binary mixture option of the Liquid Viscosity Property program.

Entering Data for Binary Mixture Viscosity

If you select the binary mixture option, the following display appears.

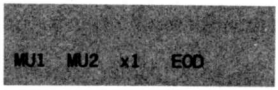


You can check the current entries by pressing INV ⟨RO1⟩ or INV ⟨RO2⟩. To enter the densities:

1. Enter the value for the density of the first liquid in grams per cm^3 and press ⟨RO1⟩.
2. Enter the value for the density of the second liquid in grams per cm^3 and press ⟨RO2⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.

Entering Data for Binary Mixture Viscosity (Continued)

After you enter the densities, the program displays:



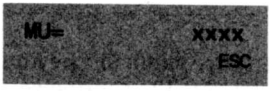
The number displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨MU1⟩, INV ⟨MU2⟩, or INV ⟨x1⟩. To enter the viscosities and the mole fraction:

1. Enter the value for the viscosity of the first liquid in centipoise and press ⟨MU1⟩.
2. Enter the value for the viscosity of the second liquid in centipoise and press ⟨MU2⟩.
3. Enter the mole fraction of the first liquid and press ⟨x1⟩. The program determines the mole fraction of the second liquid because the sum of mole fractions must be 1.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Obtaining the Binary Mixture Result

After you enter the data for the binary mixture viscosity, the following display appears.



where xxxx is the value for viscosity in centipoise.

Example: Estimating Liquid Viscosity

The following example illustrates how to use the Liquid Viscosity Property program.

Example

Estimate the viscosity of n-pentane (compound 6) at 10 °C and 100 °C. The density is 0.54 g/cm^3. n-pentane has the structural formula:

$CH_3-(CH_2)_3-CH_3$

Therefore, the group contributions for the Thomas theta parameter are

$5(-0.462)+12(0.249)=0.678.$

Procedure	Press	Display
Select the program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨LIQ⟩ ⟨MU⟩	LIQUID VISCOSITY
Select hydrocarbon	⟨HC⟩	HYDROCARBON
Specify the liquid and its temperature	6 ⟨#⟩ 10 ⟨t⟩ ⟨EOD⟩ ⟨EOD⟩	0.7
Enter the density	.54 ⟨RHO⟩	RHO= 0.54
Enter the group contributions	.678 ⟨TH⟩ ⟨EOD⟩	MU= 0.24
Repeat program with a different temperature	⟨ESC⟩ ⟨HC⟩ 100 ⟨t⟩ ⟨EOD⟩ ⟨EOD⟩	72.151
Accept the properties for the higher temperature ratio	⟨EOD⟩	MU= 0.117

Note: The literature value for the liquid viscosity of n-pentane at 100 °C is 0.131 centipoise. The estimated value has an error of 10.69%. For the compounds tested with this program, the average error was 4.14%.

Liquid Thermal Conductivity Introduction

The Liquid Thermal Conductivity Property program estimates the thermal conductivity of pure liquids using the Robbins-Kingrea method and of mixtures using the Power Law rule.

Method of Estimation—Pure Liquids

For pure liquids, the method of Robbins and Kingrea[1] is used to estimate thermal conductivity. This method uses an estimated entropy of vaporization

$$\Delta S^* = H_{vb}/T_b + R \ln(273/T_b)$$

to calculate the liquid thermal conductivity:

$$\lambda_L = \frac{(88.0 - 4.94H)(10^{-3})}{\Delta S^*} \left(\frac{0.55}{T_r}\right) C_p \rho^{4/3}$$

Here the parameter H depends on the chemical structure of the compound. H is calculated using group-contribution parameters from the "Table of H Factors" in this chapter.

Method of Estimation—Mixtures

For liquid mixtures, the Power Law mixing rule is used:

$$\lambda_m{}^{-2} = \sum_{j=1}^{n} w_j \lambda_j{}^{-2}$$

where w_j is the weight fraction of component j.

The method is a corresponding-states one,[2] limited to a temperature range of $0.4 < T_r < 0.9$. As used here, the program requires that the liquid density at 20 °C be less that 1.0 g/cm^3. For liquids with higher densities, the estimated thermal conductivity should be multiplied by the factor $T_r/0.55$. Pressure corrections on the thermal conductivity are not considered in this program.

References

[1] Robbins, L. A., and Kingrea, C. L. 1962. Estimate Thermal Conductivity. *Hydrocarbon Processing* 5: 133.

[2] Reid, R. C.; Prausnitz, J. M.; and Sherwood, T. K. 1977. *Properties of Gases and Liquids*. 3rd ed. (citing Orrick, C., and Erbar, J. H.). New York: McGraw-Hill.

The following procedure provides instructions for using the Liquid Thermal Conductivity Property program.

Before You Select the Program

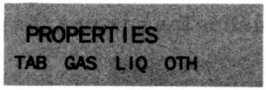
Before you select this program, you need values for heat of vaporization, specific heat, and density.

- If you do not have the value for heat of vaporization, obtain it from the latent heat of vaporization program (page 5–19) before selecting this program.
- If you do not have the value for specific heat, obtain it from the specific heat program (page 6–21) before selecting this program.
- If you do not have the value for density, obtain it from the liquid density program (page 4–26) before selecting this program.

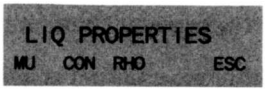
Selecting the Program

To select the Liquid Thermal Conductivity Property program:

1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨LIQ⟩. The program displays:



3. Select ⟨CON⟩.

Defining the Mixture

After you select the program, the following display appears.

```
THERMAL CON LIQ
n    t    EOD      ESC
```

You can check the current entries by pressing INV ⟨n⟩ or INV ⟨t⟩. To define the mixture:

1. Enter the number of compounds in the mixture and press ⟨n⟩.
2. Enter the value for system temperature in °C and press ⟨t⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.

Entering a Component Liquid

After you define the mixture, the program displays:

```
#( 1)
ENT  EOD          ESC
```

To specify a component liquid:

1. Enter the number of the compound for this component and press ⟨ENT⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."
2. Press ⟨EOD⟩ to proceed with the program.

Entering the Properties

After you enter the first component, the program displays:

```
COMPONENT( 1)
tc   tb   H    HVB  -->
```

Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You must supply values for H, Hvb, Cp, and RHO. You can generally accept the values for tc, tb, and Mw without checking them.

You can check the current entries by pressing INV ⟨tc⟩, INV ⟨tb⟩, INV ⟨H⟩, or INV ⟨Hvb⟩. To enter the properties:

1. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.

2. If you want to change the value for the boiling temperature, enter the new value in °C and press ⟨tb⟩.

3. Enter the H factor (listed in the Table of H Factors on page 4-24) and press ⟨H⟩.

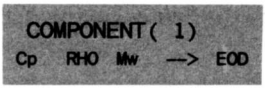
4. Enter the value for heat of vaporization at boiling temperature in calories per gram and press ⟨Hvb⟩.

5. If you enter an incorrect value, enter the correct value and press the corresponding key.

6. Press ⟨-->⟩ to display additional selections shown on the next page.

(continued)

Entering the Properties (Continued)



You can check the current entries by pressing [INV] ⟨Cp⟩, [INV] ⟨RHO⟩, or [INV] ⟨Mw⟩. To continue entering the properties:

7. Enter the value for specific heat in calories per gram-°C and press ⟨Cp⟩.

8. Enter the value for density in grams per cm^3 and press ⟨RHO⟩.

9. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.

10. If you enter an incorrect value, enter the correct value and press the corresponding key.

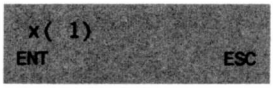
11. If you want to review the entries from the preceding page, press ⟨-->⟩.

12. Press ⟨EOD⟩ to proceed with the program.

The program repeats the entry sequence for each component.

Entering the Mole Fractions

After you enter the properties of the last component, the program prompts you to enter the mole fraction for each component except the last.



To enter a mole fraction:

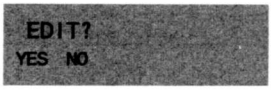
1. Enter a value for the mole fraction of this component and press ⟨ENT⟩.

2. Repeat step 1 for each component except the last.

Because the total of all the mole fractions of a mixture must be one, the program determines the last mole fraction without your entering it.

Editing the Mole Fractions

After the program determines the last mole fraction, it displays:

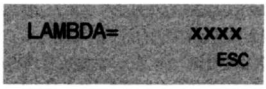


- If you want to edit a value, press ⟨YES⟩ and return to the top of this page.

- If you do not want to edit any values, press ⟨NO⟩.

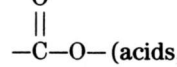
Obtaining the Result

After you select not to edit, the program presents the result.



where xxxx is the thermal conductivity expressed in calories per cm-second-°C.

Table of H Factors

	Functional Group	Number of Groups	H
Unbranched Hydrocarbons	Paraffins		0
	Olefins		0
	Rings		0
	CH_3 branches	1	1
		2	2
		3	3
	C_2H_5 branches	1	2
	i-C_3H_7 branches	1	2
	C_4H_9 branches	1	2
	F substitutions	1	1
		2	2
	Cl substitutions	1	1
		2	2
		3 or 4	3
	Br substitutions	1	4
		2	6
	I substitutions	1	5
	OH substitutions	1 (iso)	1
		1 (normal)	−1
		2	0
		1 (tertiary)	5
Oxygen Substitutions	(ketones, aldehydes)		0
	 (acids, esters)		0
	—O— (ethers)		2
NH_2 Substitutions		1	1

Source

Reid, R. C.; Prausnitz, J. M.; and Sherwood, T. K. 1977. *Properties of Gases and Liquids*. 3rd ed. (citing Orrick, C., and Erbar, J. H.). New York: McGraw-Hill.

Example: Estimating Liquid Thermal Conductivity

The following example illustrates how to use the Liquid Thermal Conductivity Property program.

Example

Estimate the liquid thermal conductivity of n-pentane (compound 6) at 0 °C.

$\rho = 0.644$ g/cm^3
Hvb at tb = 84.6 cal/g Cp = 0.536 cal/g-°C

The chemical structure of n-pentane is:

$CH_3—(CH_2)_3—CH_3$

From the Table of H Factors, the value of H for unbranched paraffin is 0.

Procedure	Press	Display
Select the program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨LIQ⟩ ⟨CON⟩	THERMAL COND LIQ
Define the mixture	1 ⟨n⟩ 0 ⟨t⟩ ⟨EOD⟩	#(1)
Enter the compound	6 ⟨ENT⟩ ⟨EOD⟩	
Enter the missing properties	0 ⟨H⟩ 84.6 ⟨Hvb⟩ ⟨-->⟩ .536 ⟨Cp⟩ .644 ⟨RHO⟩	RHO = 0.664
Accept the other properties	⟨EOD⟩	LAMBDA = 0.000306

The thermal conductivity is 0.000306 cal/cm-sec-°C.

Note: The literature value of liquid thermal conductivity of n-pentane at 0 °C is 0.000289 cal/cm-sec-°C. The program's estimated value has an error of −5.88%. For the compounds tested with this program, the average error was −1.18%.

Liquid Density Introduction

This section assists you in using the Liquid Density Property program to predict saturated liquid density for pure liquids and mixtures.

Method of Estimation for Pure Liquids

For pure liquids, this program estimates saturated liquid density using the empirical equation developed by Rackett[1,2] and generalized by Spencer and his co-workers[3,4]. The Rackett equation uses a pseudo-corresponding-states approach:

$$1/\bar{\rho}_s = [RT_c/P_c]Z_{RA}^{[1+(1-T_r)^{2/7}]}$$
$$\rho_s = \bar{\rho}_s M_w$$

$$Z_{RA} = \sum_{i=1}^{n} x_i Z_{RAi}$$

This approach depends on an empirical parameter, Z_{RA}, which is compound specific.

Method of Estimation for Mixtures

For liquid mixtures, the same equation applies but with the mixture parameters defined as

$$T_{c_m} = \sum_{i=1}^{n} x_i T_{ci} \qquad \text{(Kay's Method)}$$

$$M_{w_m} = \sum_{i=1}^{n} x_i M_{wi}$$

where x_i is the mole fraction of component i.

References

[1] Rackett, H. G. 1970. Equation of State for Saturated Liquids. *Journal of Chemical and Engineering Data* 4: 514.

[2] Rackett, H. G. 1971. Calculation of the Bubble-Point Volumes of Hydrocarbon Mixtures. *Journal of Chemical and Engineering Data* 3: 308.

[3] Spencer, C. F., and Danner, R. P. 1978. Prediction of Bubble-Point Density of Mixtures. *Journal of Chemical and Engineering Data* 2: 230.

[4] Spencer, C. F., and Alder, S. B. 1978. A Critical Review of Equations for Predicting Saturated Liquid Density. *Journal of Chemical and Engineering Data* 1: 82.

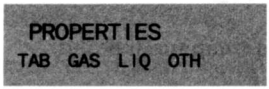
The Liquid Density Property Program

The following procedure provides instructions for using the Liquid Density Property program.

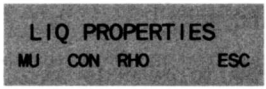
Selecting the Program

To select the Liquid Density Property program:

1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:



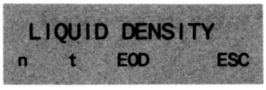
2. Select ⟨LIQ⟩. The program displays:



3. Select ⟨RHO⟩.

Defining the Mixture

After you select the program, the following display appears.

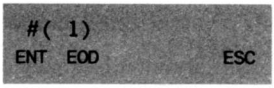


You can check the current entries by pressing [INV] ⟨n⟩ or [INV] ⟨t⟩. To define the mixture:

1. Enter the number of compounds in the mixture and press ⟨n⟩.
2. Enter the value for system temperature in °C and press ⟨t⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.

Entering a Component Liquid

After you define the mixture, the program displays:



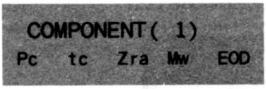
To specify a component liquid:

1. Enter the number of the compound for this component and press ⟨ENT⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."

2. Press ⟨EOD⟩ to proceed with the program.

Entering the Properties

After you enter the first component, the program displays:



Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the values for Pc, tc, Zra, and Mw without checking them.

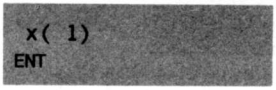
You can check the current entries by pressing INV ⟨Pc⟩, INV ⟨tc⟩, INV ⟨Zra⟩, or INV ⟨Mw⟩. To enter the properties:

1. If you want to change the value for critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.
2. If you want to change the value for critical temperature, enter the new value in °C and press ⟨tc⟩.
3. If you want to change the value for Rackett's compressibility, enter the new value and press ⟨Zra⟩.
4. If you want to change the value for molecular weight, enter the new value and press ⟨Mw⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩.

   - If the liquid is a pure substance (one component), go to "Obtaining the Result" on the next page.
   - If the liquid is a mixture of more than one component, repeat the component entry sequence on the previous page until you have entered the properties of all the components. Then go to "Entering the Mole Fractions" on the next page.

Entering the Mole Fractions

After you enter the properties of the last component, the program prompts you to enter the mole fraction for each component except the last.



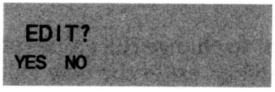
To enter a mole fraction:

1. Enter a value for the mole fraction of this component and press ⟨ENT⟩.
2. Repeat step 1 for each component except the last.

Because the total of all the mole fractions of a mixture must be one, the program determines the last mole fraction without your entering it.

Editing the Mole Fractions

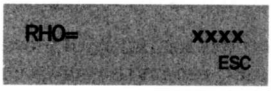
After the program determines the last mole fraction, it displays:



- If you want to edit a value, press ⟨YES⟩ and return to the top of this page.
- If you do not want to edit any values, press ⟨NO⟩.

Obtaining the Result

After you select not to edit or after you enter the properties of a single-component mixture, the program displays the result.



where xxxx is the density expressed in grams per cm^3.

Example: Estimating Liquid Density

The following example illustrates how to use the Liquid Density Property program.

Example

Estimate the density of n-pentane (compound 6) at 0 °C.

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨LIQ⟩ ⟨RHO⟩	LIQUID DENSITY
Define the mixture	1 ⟨n⟩ 0 ⟨t⟩ ⟨EOD⟩	#(1)
Enter the compound and view the density	6 ⟨ENT⟩ ⟨EOD⟩ ⟨EOD⟩	RHO = 0.644

Note: The literature value for the density of n-pentane at 0 °C is 0.6455 grams per cm^3. The estimated value has an error of 0.23%.

Chapter 5: Other Chemical Properties

This chapter describes how to use the Vapor Pressure and Raoult's Law K-Value Program, the Critical Properties program, and the Latent Heat of Vaporization Property program.

Table of Contents

Vapor Pressure and Raoult's Law K-Value Introduction

This section assists you in using the Vapor Pressure and Raoult's Law K-Value program, which estimates vapor pressure using the Frost-Kalkwarf-Thodos method. The program also estimates Raoult's Law K-values.

Method of Estimation—Vapor Pressure

The PvK program estimates vapor pressure of a compound at any temperature below the critical temperature using the Frost-Kalkwarf-Thodos[1,2] equation. You must supply the normal boiling point at one atmosphere so that the program can calculate the empirical parameter.

$$B = \frac{\ln P_c + 2.67 \ln T_{br} + 0.421875[(1/P_c T_{br}^2) - 1]}{1 - 1/T_{br} - 0.7816 \ln T_{br}}$$

Given a value for B, the vapor pressure is

$$P_v = (P_{vr})(P_c)$$

where

$$\log P_{vr} = \left(\frac{B}{T_c}\right)\left(\frac{1}{T_r} - 1\right) + \left(1.8\frac{B}{T_c} + 2.67\right)\log T_r + 0.1832\left(\frac{P_{vr}}{T_r^2} - 1\right)$$

Method of Estimation—Raoult's Law K-Value

The program also calculates the Raoult's Law K-value for the compound, given temperature and pressure:

$$K = P_v / P_{TOTAL}$$

Note: The Raoult's Law K-values should never be used for design calculations if the total pressure exceeds 15 atmospheres. Also, the K-values are not accurate for nonideal mixtures.

References

[1] Frost, A. A., and Kalkwarf, D. R. 1953. A Semi-Empirical Equation for the Vapor Pressure of Liquids as a Function of Temperature. *Journal of Chemical Physics* 2: 264.

[2] Reynes, E. G., and Thodos, G. 1962. A Reduced State Vapor-Pressure Relationship and Its Application to Hydrocarbons. *AIChE Journal* 3: 357.

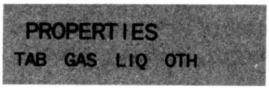
The Vapor Pressure and Raoult's Law K-Value Program

The following procedure provides instructions for using the Vapor Pressure and Raoult's Law K-Value program.

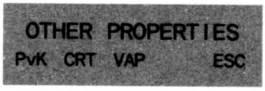
Selecting the Program

To select the Vapor Pressure and Raoult's Law K-Value program:

1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:



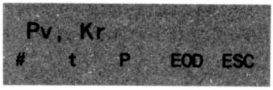
2. Select ⟨OTH⟩. The program displays:



3. Select ⟨PvK⟩.

Specifying a Compound and Its Conditions

After you select the program, the following display appears.

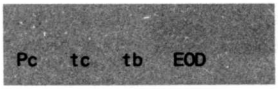


You can check the current entries by pressing INV ⟨#⟩, INV ⟨t⟩, or INV ⟨P⟩. To specify a compound and its conditions:

1. Enter the number of the compound and press ⟨#⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."
2. Enter a value for the temperature in °C and press ⟨t⟩.
3. Enter a value for the pressure in atmospheres and press ⟨P⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Entering the Properties

After you specify the compound and its conditions, the program displays:



The number displayed when this menu first appears is the last value generated (tb).

Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the values for Pc, tc, and tb without checking them.

You can check the current entries by pressing INV ⟨Pc⟩, INV ⟨tc⟩, or INV ⟨tb⟩. To enter the properties:

1. If you want to change the value for the critical pressure, enter the new value in atm and press ⟨Pc⟩.

2. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.

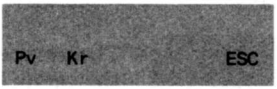
3. If you want to change the value for the normal boiling point temperature, enter the new value in °C and press ⟨tb⟩.

4. If you enter an incorrect value, enter the correct value and press the corresponding key.

5. Press ⟨EOD⟩ to proceed with the program.

Obtaining the Results

After you enter the properties, the program displays:



The number displayed when this menu first appears is the last value generated (Kr).

〈Pv〉 Displays the vapor pressure with units of atmospheres.

〈Kr〉 Displays the Raoult's Law K-value.

View each result that you want to see by pressing the key that corresponds to that result.

Example: Estimating Pv and Kr

The following example illustrates how to use the Vapor Pressure and Raoult's Law K-value program.

Example

Estimate the vapor pressure and Raoult's Law K-value of n-pentane (compound 6) at 100 °C and 1.4 atmospheres.

Procedure	Press		Display
Select program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨OTH⟩ ⟨PvK⟩	Pv, Kr	
Enter the compound and conditions	6 ⟨#⟩ 100 ⟨t⟩ 1.4 ⟨P⟩ ⟨EOD⟩		36.05
Accept the properties generated by the program	⟨EOD⟩		4.1821
View the vapor pressure and Raoult's Law K-value	⟨Pv⟩ ⟨Kr⟩	Pv = Kr =	5.8549 4.1821

Note: The literature value of the vapor pressure for n-pentane at 100 °C is 5.986 atm. The estimate contains an error of 2.19%. For the compounds tested with this program, the average error of estimations was 2.31%.

Critical Properties Introduction

The Critical Properties program estimates critical temperature, pressure, and volume using Lydersen's method. This program estimates the critical properties of a substance without using the built-in table of compounds.

Method of Estimation

This program uses Lydersen's method to estimate critical temperature, critical pressure, and critical volume. You must supply the normal boiling point at one atmosphere and the molecular weight. From the molecular structure of the compound and the Table of Increments, you determine the deltas in temperature, pressure, and volume.

Group Contributions

Lydersen's method uses the technique of group contributions based on chemical structural units to estimate the critical properties. The contributions for each structural unit are listed in the Table of Increments in this chapter.

Calculation of Critical Properties

The critical properties are calculated using the expressions

$$T_c = T_b[0.567 + \Sigma\Delta_T - (\Sigma\Delta_T)^2]^{-1}$$

$$P_c = M_W[0.34 + \Sigma\Delta_P]^{-2}$$

$$V_c = 40 + \Sigma\Delta_V$$

Summations for each property are based on the number of different structures present and the number of times an individual structure occurs in the molecule.

Reference

Lydersen, A. L. 1955. Estimation of Critical Properties of Organic Compounds. *University of Wisconsin College of Engineering Experiment Station Report Number 3*, April.

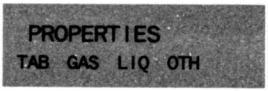
The Critical Properties Program

The following procedure provides instructions for using the Critical Properties program.

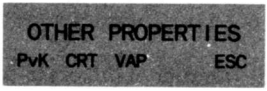
Selecting the Program

To select the Critical Properties program:

1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:



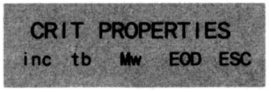
2. Select ⟨OTH⟩. The program displays:



3. Select ⟨CRT⟩.

Defining the Molecule

After you select the program, the following display appears.

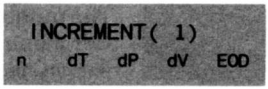


You can check the current entries by pressing INV⟨inc⟩, INV⟨tb⟩, or INV⟨Mw⟩. To define the molecule:

1. Use the increments listed in the Table of Increments on page 5-13 to construct your molecule.
2. Enter the number of different increments that comprise the molecule and press ⟨inc⟩.
3. Enter a value for the boiling temperature and press ⟨tb⟩.
4. Enter a value for the molecular weight and press ⟨Mw⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ to proceed with the program.

Entering an Increment

After you define the molecule, the program prompts you to enter information about the first type of increment.

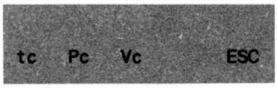


You can check the current entries by pressing INV⟨n⟩, INV⟨dT⟩, INV⟨dP⟩, or INV⟨dV⟩. To enter an increment:

1. Enter the number of occurrences of this increment and press ⟨n⟩.
2. Enter a value for the temperature delta and press ⟨dT⟩.
3. Enter a value for the pressure delta and press ⟨dP⟩.
4. Enter a value for the specific volume delta and press ⟨dV⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ to proceed with the program.
7. Repeat steps 1 through 6 for each type of increment.

Obtaining the Result

After you enter the last increment, the program displays:



The number displayed when this menu first appears is the last value generated (Vc).

⟨tc⟩ Displays the value for the critical temperature in °C.

⟨Pc⟩ Displays the value for the critical pressure in atmospheres.

⟨Vc⟩ Displays the value for the critical specific volume in cm^3/g-mole.

View each result that you want to see by pressing the key that corresponds to that result.

Table of Increments

The following table is essential in using Lydersen's method to calculate critical properties. Delta T is required in calculating tc, delta P is required in calculating Pc, and delta V is required in calculating Vc.

Nonring Increments

Type of Increment	delta T	delta P	delta V
$-CH_3$	0.020	0.227	55
$-CH_2-$	0.020	0.227	55
$-CH(-)$	0.012	0.210	51
$-C(-)(-)-$	0.000	0.210	41
$=CH_2$	0.018	0.198	45
$=CH-$	0.018	0.198	45
$=C(-)-$	0.000	0.198	36
$=C(-)-$	0.000	0.198	36
$\equiv CH$	0.005	0.153	(36)
$\equiv C-$	0.005	0.153	(36)

(continued)

Table of Increments (Continued)

	Type of Increment	delta T	delta P	delta V
Ring Increments	$-CH_2-$	0.013	0.184	44.5
		0.012	0.192	46
		(−0.007)	(0.154)	(31)
		0.011	0.154	37
		0.011	0.154	36
	=C=	0.011	0.154	36
Halogen Increments	−F	0.018	0.224	18
	−Cl	0.017	0.320	49
	−Br	0.010	(0.50)	(70)
	−I	0.12	(0.83)	(95)

	Type of Increment	delta T	delta P	delta V
Oxygen Increments	—OH (alcohols)	0.082	0.06	(18)
	—OH (phenols)	0.031	(−0.02)	(3)
	—O— (nonring)	0.021	0.16	20
	—O— (ring)	(0.014)	(0.12)	(8)
		0.040	0.29	60
		(0.033)	(0.2)	(50)
		0.048	0.33	73
	—COOH (acid)	0.085	(0.4)	80
	—COO— (ester)	0.047	0.47	80
	=O (except for combinations above)	(0.02)	(0.12)	(11)
Sulfur Increments	—SH	0.015	0.27	55
	—S— (nonring)	0.015	0.27	55
	—S— (ring)	(0.008)	(0.24)	(45)
	=S	(0.003)	(0.24)	(47)

(continued)

	Type of Increment	delta T	delta P	delta V
Nitrogen Increments	$-NH_2$	0.031	0.095	28
	$-\overset{\vert}{N}H$(nonring)	0.031	0.135	(37)
	$-\overset{\vert}{N}H$(ring)	(0.024)	(0.09)	(27)
	$-\overset{\vert}{N}-$ (nonring)	0.014	0.17	(42)
	$-\overset{\vert}{N}-$ (ring)	(0.007)	(0.13)	(32)
	$-CN$	(0.060)	(0.36)	(80)
	$-NO_2$	(0.055)	(0.42)	(78)
Miscellaneous	$-\overset{\vert}{\underset{\vert}{Si}}-$	0.03	(0.54)	—
	$-\overset{\vert}{\underset{\vert}{B}}-$	(0.03)	—	—
	$\diagdown/$ (common to two condensed saturated rings) $\overset{\vert}{C}-H$	[0.064]	—	—

Notes About the Table

- There are no increments for hydrogen.
- All bonds shown as free are connected with atoms other than hydrogen.
- You must supply the program with values for delta T, delta P, and delta V. Deltas for which a "—" is shown mean you cannot use the program to generate the corresponding critical property.
- Values in parentheses are based upon too few experimental values to be reliable.
- The value in brackets is derived from vapor-pressure measurements and a calculation technique similar to Fishtine.
- The error for T_c is usually less than 2%, but may rise to 5% for higher molecular-weight (>100) nonpolar materials. Error is uncertain for molecules with multifunctional polar groups such as glycols.
- The error for P_c is approximately twice the error of T_c.
- The error for V_c is similar to the error for P_c, but has greater variation.

Example: Estimating Critical Properties

The following example illustrates how to use the Critical Properties program.

Example

Estimate the critical properties of n-pentane.

tb = 36.2 °C
Mw = 72.151

The structural formula is

$CH_3-(CH_2)_3-CH_3$.

The molecule has two increments, CH_3- and $-CH_2-$. The CH_3- increment occurs twice, and the $-CH_2-$ increment occurs three times.

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨OTH⟩ ⟨CRT⟩	CRIT PROPERTIES
Define the molecule	2 ⟨inc⟩ 36.2 ⟨tb⟩ 72.151 ⟨Mw⟩ ⟨EOD⟩	INCREMENT(1)
Enter the first increment properties	2 ⟨n⟩ .02 ⟨dT⟩ .227 ⟨dP⟩ 55 ⟨dV⟩ ⟨EOD⟩	INCREMENT(2)
Enter the second increment properties	3 ⟨n⟩ .02 ⟨dT⟩ .227 ⟨dP⟩ 55 ⟨dV⟩ ⟨EOD⟩	315.
View the critical properties	⟨tc⟩	tc = 197.7
	⟨Pc⟩	Pc = 33.2
	⟨Vc⟩	Vc = 315.

Note: These values compare favorably with those obtained for n-pentane from the properties table program:

tc = 196.5 °C Pc = 33.24 atm Vc = 304 cm^3/g-mole.

Latent Heat of Vaporization Introduction

The Latent Heat of Vaporization Property program estimates latent heat of vaporization using the Riedel-Plank-Miller method.

Method of Estimation

The method of estimation used in this program is the Riedel-Plank-Miller vapor-pressure equation[1], based on a corresponding-states form of the Clausius-Clapeyron equation.

The program uses the normal boiling point, T_b, to calculate a reduced boiling temperature and a number of empirical parameters.

$$T_{br} = T_b/T_c$$
$$a = (T_{br} \ln P_c)/(I - T_{br})$$
$$G = 0.2471 + 0.1965a$$
$$k' = [a/2.303G - (1 + T_{br})]$$
$$T_r = T/T_c$$

It estimates the difference between the saturated gas and saturated liquid compressibility factors at the normal boiling point by the relation

$$\Delta Z_{vb} = [1 - 1/(P_c T_{br}^{3})]^{1/2}$$

The latent heat of vaporization at the normal boiling point is then calculated from the equation

$$\Delta H_{vb} = 4.57606 G T_c \Delta Z_{vb} [1 + T_{br}^{2} + k'(1 + 2T_{br})]$$

Temperature Effect

To account for the effect of temperature on the latent heat of vaporization, the program uses the Watson correlation[2] in the form

$$\Delta H_{vT} = \Delta H_{vb}[(1 - T_r) / (1 - T_{br})]^n$$

where

$$n = \begin{cases} 0.3 & T_{br} < 0.57 \\ 0.74\,T_{br} - 0.116 & 0.57 \leqslant T_{br} \leqslant 0.71 \\ 0.41 & 0.71 < T_{br} \end{cases}$$

References

[1] Reid, R. C., and Sherwood, T. K. 1966. *The Properties of Gases and Liquids*. 2nd ed. New York: McGraw-Hill.

[2] Watson, K. M. 1943. Thermodynamics of the Liquid State. *Industrial and Engineering Chemistry* 35: 398.

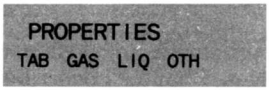
The Latent Heat of Vaporization Property Program

The following procedure provides instructions for using the Latent Heat of Vaporization Property program.

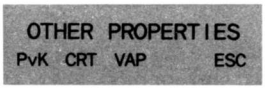
Selecting the Program

To select the Latent Heat of Vaporization Property program:

1. Select ⟨PRP⟩ from the **CHEM ENGINEERING** menu. The program displays:



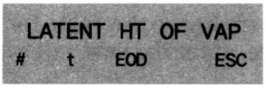
2. Select ⟨OTH⟩. The program displays:



3. Select ⟨VAP⟩.

Specifying a Compound

After you select the program, the following display appears.



You can check the current entries by pressing [INV] ⟨#⟩ or [INV] ⟨t⟩. To specify the compound and its temperature:

1. Enter the number of the compound and press ⟨#⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."

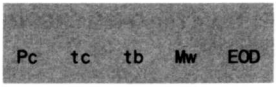
2. Enter the system temperature in °C and press ⟨t⟩.

3. If you enter an incorrect value, enter the correct value and press the corresponding key.

4. Press ⟨EOD⟩ to proceed with the program.

Entering the Properties

After you specify the compound and its conditions, the program displays:



The number displayed when this menu first appears is the last value generated (Mw).

Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the values for Pc, tc, tb, and Mw without checking them.

You can check the current entries by pressing INV ⟨Pc⟩, INV ⟨tc⟩, INV ⟨tb⟩, or INV ⟨Mw⟩. To enter the properties:

1. If you want to change the value for the critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.

2. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.

3. If you want to change the value for the boiling temperature, enter the new value in °C and press ⟨tb⟩.

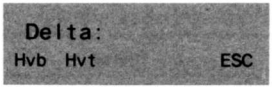
4. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.

5. If you enter an incorrect value, enter the correct value and press the corresponding key.

6. Press ⟨EOD⟩ to proceed with the program.

Obtaining the Results

After you enter the properties, the program displays:



⟨Hvb⟩ Displays the heat of vaporization at the normal boiling temperature in calories per gram.

⟨Hvt⟩ Displays the heat of vaporization for the given temperature in calories per gram.

View each result that you want to see by pressing the key that corresponds to that result.

Example: Estimating Latent Heat of Vaporization

The following example illustrates how to use the Latent Heat of Vaporization Property program.

Example

Estimate the latent heat of vaporization for n-pentane at 100 °C.

Procedure	Press	Display	
Select program	RUN ⟨CHE⟩ ⟨PRP⟩ ⟨OTH⟩ ⟨VAP⟩	LATENT HT OF VAP	
Specify the compound and enter the properties	6 ⟨#⟩ 100 ⟨t⟩ ⟨EOD⟩ ⟨EOD⟩	Delta:	
View the heats of vaporization	⟨Hvb⟩ ⟨Hvt⟩	Hvb = Hvt =	84.6 70.

Note: The literature value for n-pentane is 70.3 cal/g at 100 °C. The error in estimation is 0.43%. For the compounds tested with this program, the average error was −1.87%.

Chapter 6: Thermodynamics

This chapter describes how to use the Soave-Redlich-Kwong Thermodynamics program, the Peng-Robinson Thermodynamics program, and the Specific Heat program.

Table of Contents

Soave-Redlich-Kwong Thermodynamics Introduction

The Soave-Redlich-Kwong Thermodynamics program calculates the compressibility factor and the saturated vapor density for a pure component or mixture. It also computes fugacity coefficients for mixtures. The program takes into account the presence of hydrogen.

Method of Estimation for a Compound

The program uses the Soave[1] modification of the Redlich-Kwong equation of state:

$$Z = \frac{v}{v-b} - \frac{\alpha a}{RT(v+b)}$$

where

$$a = 0.42747\, R^2 T_c^{\,2}/P_c$$
$$b = 0.08664\, RT_c/P_c$$
$$\alpha = [1 + S(1 - \sqrt{T_r})]^2$$
$$S = 0.48508 + 1.55171\omega - 0.15613\omega^2$$

The S parameter is that given by Graboski and Daubert[2].

If the acentric factor is not known for a compound, the program estimates it using the correlation of Lee and Kessler[3]:

$$\omega = \frac{(\ln P_r - 5.92714 - 6.09648/T_{br} + 1.28862 \ln T_{br} - 0.169347 T_{br}^{\,6})}{15.2518 - 15.6875/T_{br} - 13.4721 \ln T_{br} + 0.43577 T_{br}^{\,6}}$$

where

$$T_{br} = T_b/T_c$$

Method of Estimation for Mixtures

For mixtures, the a_i, b_i, and α_i are calculated as above, and the mixture parameters are given by

$$\alpha a = \Sigma\Sigma x_i x_j \alpha_{ij} a_{ij}$$
$$b = \Sigma x_j b_j$$
$$\alpha_{ij} a_{ij} = \sqrt{\alpha_i a_i \alpha_j a_j}$$

The fugacity coefficient for each component is given by

$$\ln\phi_i = \frac{b_i}{b}(Z-1) - \ln(Z-B) - \frac{A}{B}\left(\frac{2\Sigma X_i \alpha_{ij} a_{ij}}{\alpha a} - \frac{b_i}{b}\right)\ln\left(1 + \frac{B}{Z}\right)$$

where

$$A = \alpha a P/R^2T^2$$
$$B = bP/RT$$

Presence of Hydrogen

When hydrogen is present, the Graboski and Daubert[4] correlation,

$$\alpha_{H_2} = 1.202 \exp(-0.30228 T_r)$$

is used for α_{H_2}.

References

[1] Soave, G. 1972. Equilibrium Constants from a Modified Redlich-Kwong Equation of State. *Chemical Engineering Science* 6: 1197.

[2] Graboski, M. S., and Daubert, T. E. 1978. A Modified Soave Equation of State for Phase Equilibrium Calculations: 1. Hydrocarbon Systems. *Industrial and Engineering Chemistry, Process Design and Development Quarterly* 4: 443.

[3] Lee, B. I., and Kesler, M. G. 1975. A Generalized Thermodynamic Correlation Based on Three-Parameter Corresponding States. *AIChE Journal* 3: 510.

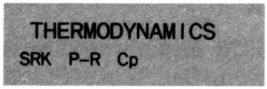
[4] Graboski, M. S., and Daubert, T. E. 1979. A Modified Soave Equation of State for Phase Equilibrium Calculations: 3. Systems Containing Hydrogen. *Industrial and Engineering Chemistry, Process Design and Development Quarterly* 2: 300.

The following procedure provides instructions for using the Soave-Redlich-Kwong Thermodynamics program.

Selecting the Program

To select the Soave-Redlich-Kwong Thermodynamics program:

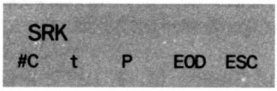
1. Select ⟨THM⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨SRK⟩.

Defining the Mixture

After you select the program, the following display appears.



You can check the current entries by pressing INV ⟨#C⟩, INV ⟨t⟩, or INV ⟨P⟩. To define the mixture:

1. Enter the number of compounds in the mixture and press ⟨#C⟩.
2. Enter the value for system temperature in °C and press ⟨t⟩.
3. Enter the value for system pressure in atmospheres and press ⟨P⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Entering the Mole Fractions

After you define the mixture, the program displays:

```
 x( 1)
ENT  EOD
```

You can check the current entry by pressing [CE]. To enter a mole fraction:

1. Enter a value for the mole fraction of this component and press ⟨ENT⟩.

2. Repeat step 1 for each component except the last.

Because the total of all the mole fractions of a mixture must be one, the program determines the last mole fraction without your entering it.

Editing the Mole Fractions

After the program determines the last mole fraction, it displays:

```
 EDIT?
YES  NO
```

- If you want to edit a value, press ⟨YES⟩ and return to the top of this page.

- If you do not want to edit any values, press ⟨NO⟩.

Entering the Component Properties

After you select not to edit, the program displays:

```
HYDROGEN?
YES  NO
```

- If hydrogen is present, press ⟨YES⟩ to designate the first component to be hydrogen.
- If hydrogen is not present, press ⟨NO⟩ to indicate that hydrogen is not in the mixture.

```
COMPONENT ( x)
#    EOD
```

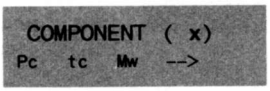
where **x** is the number of the component.

You can check the current entry by pressing INV ⟨#⟩. To specify a component liquid:

1. Enter the number of the compound for this component and press ⟨#⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."
2. Press ⟨EOD⟩ to proceed with the program.

Specifying the Properties

After you enter each component, the program displays:



Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the values for tc, Pc, and Mw without checking them.

You can check the current entries by pressing INV ⟨tc⟩, INV ⟨Pc⟩, or INV ⟨Mw⟩. To enter the properties:

1. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.

2. If you want to change the value for the critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.

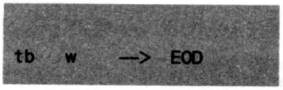
3. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.

4. If you enter an incorrect value, enter the correct value and press the corresponding key.

5. Press ⟨-->⟩ to display additional selections shown on the next page.

(continued)

Specifying the Properties (Continued)



where the message displayed when this menu first appears is left over from the previous menu

You can check the current entries by pressing INV ⟨tb⟩ or INV ⟨w⟩. To continue entering the properties:

6. If you want to change the value for the boiling temperature, enter the new value in °C and press ⟨tb⟩.

7. If you want to change the value for the acentric factor, enter the new value and press ⟨w⟩.

8. If you enter an incorrect value, enter the correct value and press the corresponding key.

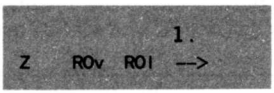
9. If you want to review the entries from the preceding page, press ⟨-->⟩.

10. Press ⟨EOD⟩ to proceed with the program.

The program repeats the entry sequence for each component.

Obtaining the Results

After you specify the properties of the last component, the program displays:



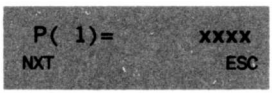
⟨Z⟩ Displays the compressibility factor of the mixture.

⟨ROv⟩ Displays the density of vapor in the mixture in grams per cm^3.

⟨ROl⟩ Displays the density of liquid in the mixture in grams per cm^3.

To obtain the results:

1. View each result that you want to see by pressing the key that corresponds to that result.
2. Press ⟨-->⟩ to proceed with the first fugacity coefficient. The program displays:



3. Press ⟨NXT⟩ to display the next fugacity coefficient.
4. Repeat step 3 for each fugacity coefficient.

Example: Estimating Compressibility and Fugacity

The following example illustrates how to use the Soave-Redlich-Kwong Thermodynamics program.

Example

Estimate the compressibility factor and the fugacity coefficient for each component of a mixture consisting of .5 mole methane (compound 1) and .5 mole ethane (compound 2), at 37.9 °C and 40.827 atm.

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨THM⟩ ⟨SRK⟩	SRK
Define the mixture	2 ⟨#C⟩ 37.9 ⟨t⟩ 40.827 ⟨P⟩ ⟨EOD⟩	x(1)
Enter the mole fraction for each component except the last	.5 ⟨ENT⟩ ⟨NO⟩	HYDROGEN?
Indicate no hydrogen is in the mixture	⟨NO⟩	COMPONENT(1)
Enter methane	1 ⟨#⟩ ⟨EOD⟩ ⟨-->⟩ ⟨EOD⟩	COMPONENT(2)
Enter ethane	2 ⟨#⟩ ⟨EOD⟩ ⟨-->⟩ ⟨EOD⟩	1.
View the results	⟨Z⟩ ⟨ROv⟩ ⟨-->⟩ ⟨NXT⟩	Z = 0.845051504 ROv = .0436517656 P(1) = 0.96727554 P(2) = 0.76233245

Note: The literature value for the compressibility factor is Z = 0.835. The calculated value is in error by −1.20%. The literature value for Phi(1) is 0.9301 and for Phi(2) is 0.7844. The calculated results are in error by −4.00% and 2.81%, respectively.

Peng-Robinson Thermodynamics Introduction

The Peng-Robinson Thermodynamics program calculates the compressibility factor, the vapor density, the vapor enthalpy, and the fugacity coefficient of each component of a mixture. If your mixture contains hydrogen, use the Soave-Redlich-Kwong Thermodynamics program instead.

Method of Calculation

The program uses the Peng-Robinson equation of state:

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+B)+b(V-b)}$$

where

$$a(T) = 0.45724(R^2T_c^{\,2}/P_c)\alpha(T_r,\omega)$$
$$b = 0.07780(RT_c/P_c)$$
$$[\alpha(T_r,\omega)]^{21/2} = 1 + K(1 - T_r^{\,1/2})$$
$$K = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

Enthalpy

The residual enthalpy of the vapor is given by

$$(H - H^*)_T = RT(Z-1) + \left(\frac{T(da/dT) - a}{2(2)^{1/2}b}\right)\ln\left(\frac{Z+2.414B}{Z-0.414B}\right)$$

where

$$B = bP/RT$$

In order to calculate the enthalpy H of a gas at a given temperature and pressure, first calculate the standard enthalpy at one atmosphere, $(H^* - H^\circ)$, and the enthalpy change, $(H - H^*)_T$ caused by a Kelvin temperature, T. Then use the expression

$$H - H^\circ = (H^* - H^\circ) + (H - H^*)_T$$

Mixtures

For mixtures,

$$a = \Sigma\Sigma x_i x_j a_i a_j$$

$$b = \Sigma x_i b_i$$

$$a_{ij} = (1 - \delta_{ij}) a_i^{1/2} a_j^{1/2}$$

where δ_{ij} is an empirical binary interaction coefficient. Though inherently less accurate, if δ_{ij} is unknown, the Peng-Robinson equation can still be used by assuming $\delta_{ij} = 0$.

Fugacity Coefficients

The fugacity coefficients are given by

$$\ln\phi_i = \frac{b_i}{b}(Z-1) - \ln(Z-B) - \frac{A}{2(2^{1/2})B}\left(\frac{2\Sigma y_i a_{ij}}{a} - \frac{b_i}{b}\right)\ln\left(\frac{Z+2.414B}{Z-0.414B}\right)$$

Reference

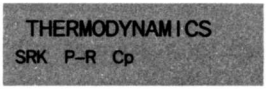
Peng, D., and Robinson, D. B. 1976. A New Two-Constant Equation of State. *Industrial and Engineering Chemistry Fundamentals Quarterly* 1: 59.

The following procedure provides instructions for using the Peng-Robinson Thermodynamics program.

Selecting the Program

To select the Peng-Robinson Thermodynamics program:

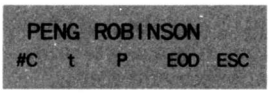
1. Select ⟨THM⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨P-R⟩.

Defining the Mixture

After you select the program, the following display appears.



You can check the current entries by pressing [INV] ⟨#C⟩, [INV] ⟨t⟩, or [INV] ⟨P⟩. To define the mixture:

1. Enter the number of compounds in the mixture and press ⟨#C⟩.
2. Enter the value for system temperature in °C and press ⟨t⟩.
3. Enter the value for system pressure in atmospheres and press ⟨P⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Entering the Mole Fractions

After you define the mixture, the program displays:

```
 x( 1)
ENT  EOD
```

You can check the current entry by pressing CE. To enter a mole fraction:

1. Enter a value for the mole fraction of this component and press ⟨ENT⟩.
2. Repeat step 1 for each component except the last.

Because the total of all the mole fractions of a mixture must be one, the program determines the last mole fraction without your entering it.

Editing the Mole Fractions

After the program determines the last mole fraction, it displays:

```
 EDIT?
YES  NO
```

- If you want to edit a value, press ⟨YES⟩ and return to the top of this page.
- If you do not want to edit any values, press ⟨NO⟩.

Entering the Component Properties

After you select not to edit, the program displays:

```
COMPONENT( x)
#    EOD
```

where x is the number of the component.

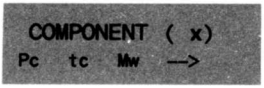
You can check the current entry by pressing INV ⟨#⟩. To specify a component:

1. Enter the number of the compound for this component and press ⟨#⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."

2. Press ⟨EOD⟩ to proceed with the program.

Specifying the Properties

After you enter each component, the program displays:



where x is the number of the component.

Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the values for Pc, tc, and Mw without checking them.

You can check the current entries by pressing INV ⟨Pc⟩, INV ⟨tc⟩, or INV ⟨Mw⟩. To enter the properties:

1. If you want to change the value for the critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.
2. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.
3. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨-->⟩ to display additional selections shown on the next page.

```
COMPONENT ( x)
tb   w    --> EOD
```

where x is the number of the component.

You can check the current entries by pressing INV ⟨tb⟩ or INV ⟨w⟩. To continue entering the properties:

6. If you want to change the value for the boiling temperature, enter the new value in °C and press ⟨tb⟩.

7. If you want to change the value for the acentric factor, enter the new value and press ⟨w⟩.

8. If you enter an incorrect value, enter the correct value and press the corresponding key.

9. If you want to review the entries from the preceding page, press ⟨-->⟩.

10. Press ⟨EOD⟩ to proceed with the program.

The program repeats the entry sequence for each component.

Entering the Interactions

After you specify the properties for the last component, the following display appears.

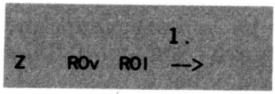
If there are no interactions, press ⟨EOD⟩ when this display appears.

You can check the current entries for i and j by pressing INV ⟨i⟩ or INV ⟨j⟩. To enter an interaction:

1. Enter a value for the first subscript (i) and press ⟨i⟩.
2. Enter a value for the second subscript (j) and press ⟨j⟩.
3. Press INV ⟨DEL⟩ to view the current entry for $delta_{ij}$.
   - ► If it is correct, press ⟨DEL⟩.
   - ► If it is not correct, enter the correct value and press ⟨DEL⟩.
4. Press ⟨EOD⟩ to proceed with the program.

Obtaining the Results

After you enter the interactions, the program displays:



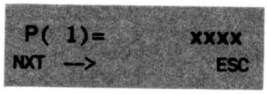
⟨Z⟩ Displays the compressibility factor of the mixture.

⟨ROv⟩ Displays the density of vapor in the mixture in grams per cm^3.

⟨ROl⟩ Displays the density of liquid in the mixture in grams per cm^3.

To obtain the results:

1. View each result that you want to see by pressing the key that corresponds to that result.
2. Press ⟨-->⟩ to proceed with the first fugacity coefficient. The program displays:



where xxxx is the fugacity coefficient.

3. Press ⟨NXT⟩ to display the next fugacity coefficient.
4. Repeat step 3 for each fugacity coefficient.

Example: Estimating Compressibility and Fugacity

The following example illustrates how to use the Peng-Robinson Thermodynamics program.

Example

Find the compressibility factor and the fugacity coefficient for each component of a mixture consisting of .5 mole methane (compound 1) and .5 mole ethane (compound 2), at 37.9 °C and 40.827 atm.

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨THM⟩ ⟨P-R⟩	PENG ROBINSON
Define the mixture	2 ⟨#C⟩ 37.9 ⟨t⟩ 40.827 ⟨P⟩ ⟨EOD⟩	x(1)
Enter the mole fraction for each component except the last	.5 ⟨ENT⟩ ⟨NO⟩	COMPONENT(1)
Enter methane	1 ⟨#⟩ ⟨EOD⟩ ⟨-->⟩ ⟨EOD⟩	COMPONENT(2)
Enter ethane	2 ⟨#⟩ ⟨EOD⟩ ⟨-->⟩ ⟨EOD⟩	ENTER DELTAs
Specify no interactions	⟨EOD⟩	0.
View the results	⟨Z⟩	Z = .8217431803
	⟨ROv⟩	ROv = .0448899255
	⟨-->⟩	P(1) = 0.94826855
	⟨NXT⟩	P(2) = 0.73954954
	⟨-->⟩	dH = −15.63554336

Note: The literature value for the compressibility factor is Z = 0.835. The calculated value is in error by 1.59%. The literature value for Phi(1) is 0.9301 and for Phi(2), 0.7844. The calculated results are in error by −1.95% and 5.72%, respectively.

Specific Heat Introduction

The Specific Heat program estimates ideal heat capacity for hydrocarbons and nonhydrocarbons in the gas and liquid phases.

Method of Estimation for Hydrocarbons

For hydrocarbon compounds, the program is based upon the empirical model developed by Yuan and Mok[1,2] to correlate ideal heat capacity data for hydrocarbons. Yuan and Mok use the exponential form:

$$Cp° = A + Be^{-C/T^n}$$

to curve fit experimental data for the ideal heat capacity. The built-in properties table supplies the curve-fit parameters A, B, C, and n, developed by Duran, Thinh, Ramalho, and Kaliaguine[3].

Method of Estimation for Nonhydrocarbons

For nonhydrocarbon compounds, the empirical polynomial model

$$Cp° = A + BT + CT^2 + DT^3$$

represents the ideal gas heat capacity. The built-in properties table supplies the curve-fit parameters A, B, C, and D, developed by Reid, Prausnitz, and Sherwood[4] for most of the compounds.

The Effect of Pressure on Gas Heat Capacity

To account for the significant effect of pressure on gas-phase heat capacity, the program uses the method of residual heat capacities of Lee and Kesler[5]. In the Lee-Kesler method, the actual gas heat capacity is related to the ideal gas heat capacity by the equation

$$Cp = Cp^{\circ} + (\Delta Cp)^{(0)} + \omega(\Delta Cp)^{(1)}$$

where $(\Delta Cp)^{(0)}$ and $(\Delta Cp)^{(1)}$ are correction terms for heat capacity and ^{0} is the Pitzer acentric factor. The simple fluid correction, $(\Delta Cp)^{(0)}$, is a function of T_r and P_r and is given in the Table of Residual Heat Capacities in this chapter. The deviation function, $(\Delta Cp)^{(1)}$, is also a function of T_r and P_r and is given in this table as well.

Liquid Heat Capacity

The program estimates liquid-phase heat capacities by using the derivative of the empirical, isothermal enthalpy-difference correlation developed by Lee and Edmister[6]. The saturated liquid heat capacity is then related to the ideal gas heat capacity.

$$\begin{aligned} C_{SL} = R(&-A_3 - 6A_4T_r^{\,2} - 42A_5T_r^{\,6} \\ &+ P_r(-A_7 - 6A_8T_r^{\,2} - 12A_9T_r^{\,3}P_r^{\,2}) \\ &+ \omega(2A_{10}T_r - 12A_{13}T_r^{\,3}P_r^{\,2})) + Cp^{\circ} \end{aligned}$$

The empirical parameters in this equation are:

$A_3 = -6.90287$ $\qquad$ $A_8 = 0.18940$

$A_4 = 1.87895$ $\qquad$ $A_9 = 0.002584$

$A_5 = -0.33448$ $\qquad$ $A_{10} = 8.7015$

$A_7 = -0.286517$ $\qquad$ $A_{13} = 0.002255$

References

[1] Yuan, S. C., and Mok, Y. I. 1968. A New Look at Heat Capacity Prediction. *Hydrocarbon Processing* 3: 133.

[2] Yuan, S. C., and Mok, Y. I. 1968. A New Look at Heat Capacity Prediction, Part 2. *Hydrocarbon Processing* 7: 153.

[3] Duran, J. L.; Thinh, T. P.; Ramalho, R. S.; and Kaliaguine, S. 1976. Predict Heat Capacity More Accurately. *Hydrocarbon Processing* 8: 153.

[4] Reid, R. C.; Prausnitz, J. M.; and Sherwood, T. K. 1977. *The Properties of Gases and Liquids*. 3rd ed. New York: McGraw-Hill.

[5] Lee, B. I., and Kesler, M. G. 1975. A Generalized Thermodynamic Correlation Based on Three-Parameter Corresponding States. *AIChE Journal* 3: 510.

[6] Lee, B. I., and Edmister, W. C. 1971. Fugacity Coefficients and Isothermal Enthalpy Differences for Pure Hydrocarbon Liquids. *Industrial and Engineering Fundamentals Quarterly* 2: 229.

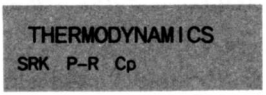
The Specific Heat Program

The following procedure provides instructions for using the Specific Heat program.

Selecting the Program

To select the Specific Heat program:

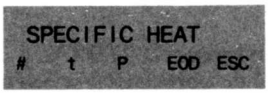
1. Select ⟨THM⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨Cp⟩.

Specifying a Compound

After you select the program, the following display appears.

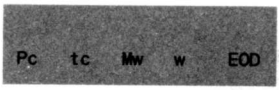


You can check the current entries by pressing [INV] ⟨#⟩, [INV] ⟨t⟩ or [INV] ⟨P⟩. To specify a compound and its conditions:

1. Enter the number of the compound and press ⟨#⟩. Chapter 1 describes this entry in "Entering the Physical Parameters of a Compound."
2. Enter a value for the temperature in °C and press ⟨t⟩.
3. Enter a value for the pressure in atmospheres and press ⟨P⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Specifying the Properties

After you specify the compound and its conditions, the program displays:



The number displayed when this menu first appears is the last value generated (Mw).

Review the properties and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the values for Pc, tc, Mw, and w without checking them.

You can check the current entries by pressing INV ⟨Pc⟩, INV ⟨tc⟩, INV ⟨Mw⟩, or INV ⟨w⟩. To enter the properties:

1. If you want to change the value for the critical temperature, enter the new value in °C and press ⟨tc⟩.

2. If you want to change the value for the critical pressure, enter the new value in atmospheres and press ⟨Pc⟩.

3. If you want to change the value for the molecular weight, enter the new value and press ⟨Mw⟩.

4. If you want to change the value for the acentric factor, enter the new value and press ⟨w⟩. The program uses this entry only if you select the pressure correction option.

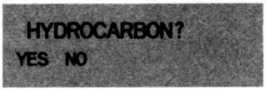
5. If you enter an incorrect value, enter the correct value and press the corresponding key.

6. Press ⟨EOD⟩ to proceed with the program.

(continued)

Specifying the Properties (Continued)

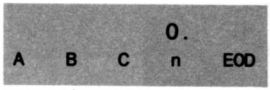
The program prompts you to indicate whether to use the hydrocarbon or the nonhydrocarbon specific heat model.



- If the hydrocarbon specific heat model applies, press ⟨YES⟩ and go to the next page.
- If the nonhydrocarbon specific heat model applies, press ⟨NO⟩ and go to page 6–28.

Entering the Hydrocarbon Coefficients

When you select the hydrocarbon specific heat model, the program displays:



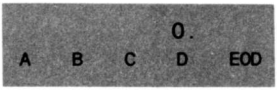
Review the coefficients and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the coefficients without checking them.

You can check the current entries by pressing INV ⟨A⟩, INV ⟨B⟩, INV ⟨C⟩, or INV ⟨n⟩. To enter the coefficients:

1. If you want to change the A coefficient, enter the new value and press ⟨A⟩.
2. If you want to change the B coefficient, enter the new value and press ⟨B⟩.
3. If you want to change the C coefficient, enter the new value and press ⟨C⟩.
4. If you want to change the n coefficient, enter the new value and press ⟨n⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ and go to page 6–29.

Entering the Nonhydrocarbon Coefficients

When you select the nonhydrocarbon specific heat model, the program displays:



Review the coefficients and decide whether to accept or to change them. Chapter 1 describes this menu in "Entering the Physical Parameters of a Compound." You can generally accept the coefficients without checking them.

You can check the current entries by pressing INV ⟨A⟩, INV ⟨B⟩, INV ⟨C⟩, or INV ⟨D⟩. To enter the coefficients:

1. If you want to change the A coefficient, enter the new value and press ⟨A⟩.
2. If you want to change the B coefficient, enter the new value and press ⟨B⟩.
3. If you want to change the C coefficient, enter the new value and press ⟨C⟩.
4. If you want to change the D coefficient, enter the new value and press ⟨D⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ to proceed with the program.

Entering a Pressure Correction

After you enter the coefficients, the program displays:

```
 PR CORRECTION?
YES NO            ESC
```

- If the compound does not need a pressure correction, press ⟨NO⟩ and go to "Obtaining the Results" on page 6–31.
- If the compound needs a pressure correction:

  1. Press ⟨YES⟩. The program displays:

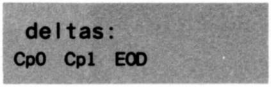
     ```
      SEE:
     Tr  Pr  -->       ESC
     ```

  2. Press ⟨Tr⟩ to display the reduced temperature.
  3. Press ⟨Pr⟩ to display the reduced pressure.
  4. Use the values of Tr and Pr to determine Cp0 and Cp1 from the Table of Residual Heat Capacity on pages 6–32 through 6–35. To arrive at values for Cp0 and Cp1 that are based on the calculated Tr and Pr usually requires you to interpolate between two rows and two columns. A pressure correction is not valid if Tr and Pr correspond to a position in the table that is marked "Undef."

(continued)

Entering a Pressure Correction (Continued)

5. Press ⟨--->. The program displays:



You can check the current entries by pressing INV ⟨Cp0⟩ or INV ⟨Cp1⟩.

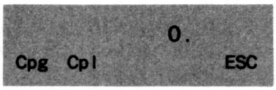
6. Enter the value for simple fluid correction (from the Table of Residual Heat Capacity) and press ⟨Cp0⟩.

7. Enter the value for the deviation function (from the Table of Residual Heat Capacity) and press ⟨Cp1⟩.

8. Press ⟨EOD⟩ and go to "Obtaining the Results" on the next page.

Obtaining the Results

After you enter a pressure correction or select not to include a pressure correction, the program displays:



〈Cpg〉 Displays the gas specific heat in calories per gram-°C.

〈Cpl〉 Displays the liquid specific heat in calories per gram-°C.

View each result that you want to see by pressing the key that corresponds to that result.

Table of Residual Heat Capacities

The following table for Cp0 is defined by the simple fluid correction function, $(Cp - Cp^0)/R$.

Tr	Pr 0.010	0.050	0.100	0.200	0.400	0.600	0.800
0.30	2.805	2.807	2.809	2.814	2.830	2.842	2.854
0.35	2.808	2.810	2.812	2.815	2.823	2.835	2.844
0.40	2.925	2.926	2.928	2.933	2.935	2.940	2.945
0.45	2.989	2.990	2.990	2.991	2.993	2.995	2.997
0.50	3.006	3.005	3.004	3.003	3.001	3.000	2.998
0.55	0.118	3.002	3.000	2.997	2.990	2.984	2.978
0.60	0.089	3.009	3.006	2.997	2.990	2.984	2.978
0.65	0.069	0.387	3.047	3.036	3.014	2.993	2.973
0.70	0.054	0.298	0.687	3.138	3.099	3.065	3.033
0.75	0.044	0.236	0.526	3.351	3.284	3.225	3.171
0.80	0.036	0.191	0.415	1.032	3.647	3.537	3.440
0.85	0.030	0.157	0.336	0.794	4.404	4.158	3.957
0.90	0.025	0.131	0.277	0.633	1.858	5.679	5.095
0.93	0.023	0.118	0.249	0.560	1.538	4.208	6.720
0.95	0.021	0.111	0.232	0.518	1.375	3.341	9.316
0.97	0.020	0.104	0.217	0.480	1.240	2.778	9.585
0.98	0.019	0.101	0.210	0.463	1.181	2.563	7.350
0.99	0.019	0.098	0.204	0.447	1.126	2.378	6.038
1.00	0.018	0.095	0.197	0.431	1.076	2.218	5.156
1.01	0.018	0.092	0.191	0.417	1.029	2.076	4.516
1.02	0.017	0.089	0.185	0.403	0.986	1.951	4.025
1.05	0.016	0.082	0.169	0.365	0.872	1.648	3.047
1.10	0.014	0.071	0.147	0.313	0.724	1.297	2.168
1.15	0.012	0.063	0.128	0.271	0.612	1.058	1.670
1.20	0.011	0.055	0.113	0.237	0.525	0.885	1.345
1.30	0.009	0.044	0.089	0.185	0.400	0.651	0.946
1.40	0.007	0.036	0.072	0.149	0.315	0.502	0.711
1.50	0.006	0.029	0.060	0.122	0.255	0.399	0.557
1.60	0.005	0.025	0.050	0.101	0.210	0.326	0.449
1.70	0.004	0.021	0.042	0.086	0.176	0.271	0.371
1.80	0.004	0.018	0.036	0.073	0.150	0.229	0.311
1.90	0.003	0.016	0.031	0.063	0.129	0.196	0.265
2.00	0.003	0.014	0.027	0.055	0.112	0.170	0.229
2.20	0.002	0.011	0.021	0.043	0.086	0.131	0.175
2.40	0.002	0.009	0.017	0.034	0.069	0.104	0.138
2.60	0.001	0.007	0.014	0.028	0.056	0.084	0.112
2.80	0.001	0.006	0.012	0.023	0.046	0.070	0.093
3.00	0.001	0.005	0.010	0.020	0.039	0.058	0.078
3.50	0.001	0.003	0.007	0.013	0.027	0.040	0.053
4.00	0.000	0.002	0.005	0.010	0.019	0.029	0.038

1.000	1.200	1.500	2.000	3.000	5.000	7.000	10.000
2.866	2.878	2.896	2.927	2.989	3.122	3.257	3.466
2.853	2.861	2.875	2.897	2.944	3.042	3.145	3.313
2.951	2.956	2.965	2.979	3.014	3.085	3.164	3.293
2.999	3.002	3.006	3.014	3.032	3.079	3.135	3.232
2.997	2.996	2.995	2.995	2.999	3.019	3.054	3.122
2.973	2.968	2.961	2.951	2.938	2.934	2.947	2.988
2.952	2.942	2.927	2.907	2.874	2.840	2.831	2.847
2.955	2.938	2.914	2.878	2.822	2.753	2.720	2.709
3.003	2.975	2.937	2.881	2.792	2.681	2.621	2.582
3.112	3.076	3.015	2.928	2.795	2.629	2.537	2.469
3.354	3.277	3.176	3.038	2.838	2.601	2.473	2.373
3.790	3.647	3.470	3.240	2.931	2.599	2.427	2.292
4.677	4.359	4.00	3.585	3.096	2.626	2.399	2.227
5.766	5.149	4.533	3.902	3.236	2.657	2.392	2.195
7.127	6.010	5.050	4.180	3.351	2.684	2.391	2.175
10.011	7.451	5.785	4.531	3.486	2.716	2.393	2.159
13.270	8.611	6.279	4.743	3.560	2.733	2.395	2.151
21.948	10.362	6.897	4.983	3.641	2.752	2.398	2.144
Undef.	13.281	7.686	5.255	3.729	2.773	2.401	2.138
22.295	18.967	8.708	5.569	3.821	2.794	2.405	2.131
13.184	31.353	10.062	5.923	3.920	2.816	2.408	2.125
6.458	20.234	16.457	7.296	4.259	2.816	2.408	2.125
3.649	6.510	13.256	9.787	4.927	3.033	2.462	2.093
2.553	3.885	6.985	9.094	5.535	3.186	2.508	2.093
1.951	2.758	4.430	6.911	5.710	3.326	2.555	2.079
1.297	1.711	2.458	3.850	4.793	3.452	2.628	2.077
0.946	1.208	1.650	2.462	3.573	3.282	2.626	2.068
0.728	0.912	1.211	1.747	2.647	2.917	2.525	2.038
0.580	0.719	0.938	1.321	2.016	2.508	2.347	1.978
0.475	0.583	0.752	1.043	1.586	2.128	2.130	1.889
0.397	0.484	0.619	0.848	1.282	1.805	1.907	1.778
0.336	0.409	0.519	0.706	1.060	1.538	1.696	1.656
0.289	0.350	0.443	0.598	0.893	1.320	1.505	1.531
0.220	0.265	0.334	0.446	0.661	0.998	1.191	1.292
0.173	0.208	0.261	0.347	0.510	0.779	0.956	1.086
0.140	0.168	0.210	0.278	0.407	0.624	0.780	0.917
0.116	0.138	0.172	0.227	0.332	0.512	0.647	0.779
0.097	0.116	0.144	0.190	0.277	0.427	0.545	0.668
0.066	0.079	0.098	0.128	0.187	0.289	0.374	0.472
0.048	0.057	0.071	0.093	0.135	0.209	0.272	0.350

Table of Residual Heat Capacities (Continued)

The following table for Cp1 is defined by the deviation function, $(Cp - Cp^1)/R$.

Tr	Pr 0.010	0.050	0.100	0.200	0.400	0.600	0.800
0.30	8.462	8.445	8.424	8.381	8.281	8.192	8.102
0.35	9.775	9.762	9.746	9.713	9.646	9.568	9.499
0.40	11.494	11.484	11.471	11.438	11.394	11.343	11.291
0.45	12.651	12.643	12.633	12.613	12.573	12.532	12.492
0.50	13.111	13.106	13.099	13.084	13.055	13.025	12.995
0.55	0.511	13.035	13.030	13.021	13.002	12.981	12.961
0.60	0.345	12.679	12.675	12.668	12.653	12.637	12.620
0.65	0.242	1.518	12.148	12.145	12.137	12.128	12.117
0.70	0.174	1.026	2.698	11.557	11.564	11.563	11.559
0.75	0.129	0.726	1.747	10.967	10.995	11.011	11.019
0.80	0.097	0.532	1.212	3.511	10.490	10.536	10.566
0.85	0.075	0.399	0.879	2.247	9.999	10.153	10.245
0.90	0.058	0.306	0.658	1.563	5.486	9.793	10.180
0.93	0.050	0.263	0.560	1.289	3.890	Undef.	10.285
0.95	0.046	0.239	0.505	1.142	3.215	9.389	9.993
0.97	0.042	0.217	0.456	1.018	2.712	6.588	Undef.
0.98	0.040	0.207	0.434	0.962	2.506	5.711	Undef.
0.99	0.038	0.198	0.414	0.911	2.324	5.027	Undef.
1.00	0.037	0.189	0.394	0.863	2.162	4.477	10.511
1.01	0.035	0.181	0.376	0.819	2.016	4.026	8.437
1.02	0.034	0.173	0.359	0.778	1.884	3.648	7.044
1.05	0.030	0.152	0.313	0.669	1.559	2.812	4.679
1.10	0.024	0.123	0.252	0.528	1.174	1.968	2.919
1.15	0.020	0.101	0.205	0.424	0.910	1.460	2.048
1.20	0.016	0.083	0.168	0.345	0.722	1.123	1.527
1.30	0.012	0.058	0.116	0.235	0.476	0.715	0.938
1.40	0.008	0.042	0.083	0.166	0.329	0.484	0.624
1.50	0.006	0.030	0.061	0.120	0.235	0.342	0.437
1.60	0.005	0.023	0.045	0.089	0.173	0.249	0.317
1.70	0.003	0.017	0.034	0.068	0.130	0.187	0.236
1.80	0.003	0.013	0.027	0.052	0.100	0.143	0.180
1.90	0.002	0.011	0.021	0.041	0.078	0.111	0.140
2.00	0.002	0.008	0.017	0.032	0.062	0.088	0.110
2.20	0.001	0.005	0.011	0.021	0.040	0.057	0.072
2.40	0.001	0.004	0.007	0.014	0.028	0.039	0.049
2.60	0.001	0.003	0.005	0.010	0.020	0.028	0.035
2.80	0.000	0.002	0.004	0.008	0.014	0.021	0.026
3.00	0.000	0.001	0.003	0.006	0.011	0.016	0.020
3.50	0.000	0.001	0.002	0.003	0.006	0.009	0.012
4.00	0.000	0.001	0.001	0.002	0.004	0.006	0.008

1.000	1.200	1.500	2.000	3.000	5.000	7.000	10.000
8.011	7.920	7.785	7.558	7.103	6.270	5.372	4.020
9.430	9.360	9.256	9.080	8.728	8.013	7.290	6.285
11.240	11.188	11.110	10.980	10.709	10.170	9.625	8.803
12.451	12.409	12.347	12.243	12.029	11.592	11.183	10.533
12.964	12.933	12.886	12.805	12.639	12.288	11.946	11.419
12.939	12.917	12.882	12.823	12.695	12.407	12.103	11.673
12.589	12.574	12.550	12.506	12.407	12.165	11.905	11.526
12.105	12.092	12.060	12.026	11.943	11.728	11.494	11.141
11.553	11.536	11.524	11.495	11.416	11.208	10.985	10.661
11.024	11.022	11.013	10.986	10.898	10.677	10.448	10.132
10.583	10.590	10.587	10.556	10.446	10.176	9.917	9.591
10.297	10.321	10.324	10.278	10.111	9.740	9.433	9.075
10.349	10.409	10.401	10.279	9.940	9.389	8.999	8.592
10.769	10.875	10.801	10.523	9.965	9.225	8.766	8.322
11.420	11.607	11.387	10.865	10.055	9.136	8.621	8.152
13.001	Undef.	12.498	11.445	10.215	9.061	8.485	7.986
Undef.	Undef.	Undef.	11.856	10.323	9.037	8.420	7.905
Undef.	Undef.	Undef.	12.388	10.457	9.011	8.359	7.826
Undef.	Undef.	Undef.	13.081	10.617	8.990	8.293	7.747
Undef.	Undef.	Undef.	Undef.	10.805	8.973	8.236	7.670
Undef.	Undef.	Undef.	Undef.	11.024	8.960	8.182	7.595
7.173	2.277	Undef.	Undef.	11.852	8.939	8.018	7.377
3.877	4.002	3.927	Undef.	Undef.	8.933	7.759	7.031
2.587	2.844	2.236	7.716	12.812	8.849	7.504	6.702
1.881	2.095	1.962	2.965	9.494	8.508	7.206	6.384
1.129	1.264	1.327	1.288	3.855	6.758	6.365	5.735
0.743	0.833	0.904	0.905	1.652	4.524	5.193	5.035
0.517	0.580	0.639	0.666	0.907	2.823	3.944	4.289
0.374	0.419	0.466	0.499	0.601	1.755	2.781	3.545
0.278	0.312	0.349	0.380	0.439	1.129	2.060	2.867
0.212	0.238	0.267	0.296	0.337	0.764	1.483	2.287
0.164	0.185	0.209	0.234	0.267	0.545	1.085	1.817
0.130	0.146	0.166	0.187	0.217	0.407	0.812	1.446
0.085	0.096	0.110	0.126	0.150	0.256	0.492	0.941
0.058	0.066	0.076	0.089	0.109	0.180	0.329	0.644
0.042	0.048	0.056	0.066	0.084	0.137	0.239	0.466
0.031	0.036	0.042	0.051	0.067	0.110	0.187	0.356
0.024	0.028	0.033	0.041	0.055	0.092	0.153	0.285
0.015	0.017	0.021	0.026	0.038	0.067	0.108	0.190
0.010	0.012	0.015	0.019	0.029	0.054	0.085	0.146

Sources

[1] Yuan, S. C., and Mok, Y. I. 1968. A New Look at Heat Capacity Prediction. *Hydrocarbon Processing* 3: 133.

[2] Yuan, S. C., and Mok, Y. I. 1968. A New Look at Heat Capacity Prediction, Part 2. *Hydrocarbon Processing* 7: 153.

Example: Estimating Specific Heat

The following example illustrates how to use the Specific Heat program.

Example

Estimate the gas and liquid specific heat of n-pentane (compound 6) at 0 °C and 1 atmosphere of pressure.

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨THM⟩ ⟨Cp⟩	SPECIFIC HEAT
Enter the compound and conditions	6 ⟨#⟩ 0 ⟨t⟩ 1 ⟨P⟩ ⟨EOD⟩	72.151
Accept the properties generated by the program	⟨EOD⟩	HYDROCARBON?
Indicate this is a hydrocarbon and accept the coefficients	⟨YES⟩ ⟨EOD⟩	PR CORRECTION?
Select pressure correction	⟨YES⟩	SEE:
View the temperature ratio and pressure ratio	⟨Tr⟩ ⟨Pr⟩ ⟨-->⟩	Tr = 0.582 Pr = 0.030 deltas:

The values for Tr and Pr do not coincide with values listed in the table. However, linear interpolation can arrive at satisfactory values for Cp0 and Cp1 by following this procedure.

1. Interpolate within the row above the value.
2. Interpolate within the row below the value.
3. Interpolate between the two preliminary interpolations.

(continued)

Example (Continued)

The portion of the Cp0 table that encompasses Tr = 0.582 and Pr = 0.03 is:

Tr	Pr 0.010	0.050	...
0.55	0.118	3.002	...
0.60	0.089	3.009	...
:	:	:	...

Procedure	Press	Display
Interpolate for Tr of .55	(.03 − .01) + (.05 − .01) × (3.002 − 0.118) + 0.118 =	1.56
Interpolate for Tr of .60	(.03 − .01) + (.05 − .01) × (3.009 − 0.089) + 0.089 =	1.549
Interpolate for Tr of .582 from the preliminary interpolations	(.582 − .60) + (.55 − .60) × (1.56 − 1.549) + 1.549 =	1.55296
Enter the interpolated value for Cp0	⟨Cp0⟩	Cp0 = 1.55296

Example (Continued)

The portion of the Cp1 table that encompasses Tr = 0.582 and Pr = 0.03 is:

	Pr		
Tr	0.010	0.050	...
0.55	0.511	13.035	...
0.60	0.345	12.679	...
:	:	:	...

Procedure	Press	Display
Interpolate for Tr of .55	(.03 − .01) + (.05 − .01) × (13.035 − 0.511) + 0.511 =	6.773
Interpolate for Tr of .60	(.03 − .01) + (.05 − .01) × (12.679 − 0.345) + 0.345 =	6.512
Interpolate for Tr of .582 from the preliminary interpolations	(.582 − .60) + (.55 − .60) × (6.773 − 6.512) + 6.512 =	6.60596
Enter the interpolated value for Cp1	⟨Cp1⟩	Cp1 = 6.60596

Example (Continued)

Procedure	Press		Display
Display the specific heats	⟨EOD⟩ ⟨Cpg⟩ ⟨Cpl⟩	Cpg = Cpl =	0.46 0.542

The gas specific heat is 0.46 calories per gram-°C, and the liquid specific heat is 0.542 calories per gram-°C.

Note: The table below summarizes the expected values for n-pentane at 0 °C, estimated values, and percent error of the specific heats.

	Literature Cp cal/g-°C	Estimated Cp cal/g-°C	Error %
gas	0.379	0.46	−21.4
liq	0.536	0.542	−1.12

For the compounds tested with this program, the average errors were:

Cp gas = 0.32%
Cp liq = −1.49%.

Chapter 7: Pipe Design for Liquid Flow

This chapter describes how to use the Pipe Design for Liquid Flow program, which calculates pressure drop or flow rate for a given pipe configuration.

Table of Contents

Pipe Design for Liquid Flow Introduction

The Pipe Design for Liquid Flow program evaluates the pressure drop for flowing liquids in a pipe when the liquid flow rate, physical properties, and a definition of the pipe geometry are given. It also calculates the liquid flow rate, given the pressure drop.

Pressure-Head Option

When the liquid flow rate is given, the program uses the liquid Reynolds number[1]

$$Re = \frac{Dv\rho}{\mu}$$

to choose the appropriate friction factor correlation.

$$f = 16/Re \qquad Re \leq 2100$$

$$f = 0.0001Re^{0.575} \qquad 2100 < Re \leq 3500$$

$$1/\sqrt{f} = -4\log\left(\frac{\epsilon}{3.7D} + \frac{2.51}{2Re\sqrt{f}}\right) \qquad 3500 < Re$$

The equivalent pipe length is found from the expression

$$L_{eq} = L + D\Sigma(Le/D)_{fittings}$$

where the Le/D for the fittings are[2]:

Fitting	Le/D
Standard 90° Elbow	32
180° Close Bend	75
Tee (entering run)	60
Tee (entering branch)	90
Open Gate Valve	7
Open Globe Valve	300

The head loss comes from the expression[3]

$$\omega_o = \Delta Z + \frac{2fv^2L_{eq}}{g_eD}$$

where ΔZ is the net difference in elevation between the pipe exit and the pipe entrance.

The total pressure drop due to liquid flow through the pipe is given by

$$\Delta P = (\omega_o\rho)/144$$

Flow Rate Option

By entering a value for the pressure drop, you select to solve for the flow rate. When the program computes the flow rate, it uses an iterative method.

First, the program assumes a friction factor, which it uses to estimate the liquid flow rate and calculate the pressure drop. It then compares the calculated pressure drop to the given pressure drop and revises the flow-rate estimate. The calculation continues until the estimated flow rate causes a pressure drop that is within 0.5% of the entered pressure drop.

References

[1] Reynolds, O. 1883. *Transactions of the Royal Society of London* A174: 35.

[2] Peters, M. S., and Timmerhaus, K. D. 1980. *Plant Design and Economics for Chemical Engineers*. 3rd ed. New York: McGraw-Hill.

[3] Welty, J. R.; Wicks, C. E.; and Wilson, R. E. 1976. *Fundamentals of Momentum Heat and Mass Transfer*. 2nd ed. New York: Wiley.

The Pipe Design for Liquid Flow Program

The following procedure provides instructions for using the Pipe Design for Liquid Flow program.

Before You Select the Program

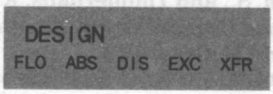
Before you select this program, you need values for density and viscosity.

- If you do not have the value for density, obtain it from the liquid density program (page 4–26) before selecting this program.
- If you do not have the value for viscosity, obtain it from the liquid viscosity program (page 4–2) before selecting this program.

Selecting the Program

To select the Pipe Design for Liquid Flow program:

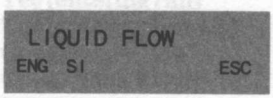
1. Select ⟨DSN⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨FLO⟩.

Selecting the Units

After you select the program, the following display appears.



- If your entries and results are to be in the English system of units, press ⟨ENG⟩.
- If your entries and results are to be in the metric (SI, System International) system of units, press ⟨SI⟩.

If you run the program with one set of units and then return to this display and select the other set of units, the numbers you entered previously are automatically converted.

Entering the Liquid Flow Data

After you specify the units, the following display appears.

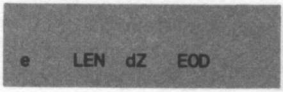
```
 LIQUID FLOW
RHO  MU   DIA  EOD  ESC
```

You can check the current entries by pressing INV ⟨RHO⟩, INV ⟨MU⟩, or INV ⟨DIA⟩. To enter the conditions of the liquid flow:

1. Enter a value for the density of the liquid in either lb/ft^3 (English) or g/cm^3 (metric). Then press ⟨RHO⟩.
2. Enter a value for the viscosity of the liquid in either lb/ft-hr (English) or centipoise (metric). Then press ⟨MU⟩.
3. Enter a value for the inside diameter of the pipe in either feet (English) or meters (metric). Then press ⟨DIA⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Entering the Pipe Characteristics

After you enter the liquid flow data, the following display appears.



where the message displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨e⟩, INV ⟨LEN⟩, or INV ⟨dZ⟩. To enter the pipe characteristics:

1. Enter a value for the roughness of the pipe in either feet (English) or meters (metric). Then press ⟨e⟩.
2. Enter a value for the length of the pipe in either feet (English) or meters (metric). Then press ⟨LEN⟩.
3. Enter a value for the change in elevation of the pipe in either feet (English) or meters (metric). A positive value for dZ indicates uphill flow and negative value indicates downhill flow. Then press ⟨dZ⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Specifying the Configuration

After you enter the pipe characteristics, the following display appears.

```
 # OF FITTINGS
NIL  T->  ->T  EOD
```

You can check the current entries by pressing INV <T->> or INV <->T>. To specify the configuration:

- If the pipe has no fittings, press <NIL>. Go to page 7–9.
- If the pipe has fittings, classify each fitting as:

  T-fitting that has one output flow (T entering run)
  T-fitting that has one input flow (T entering branch)
  90° elbow bend (L-fitting)
  180° elbow bend (U-fitting)
  Open gate valve
  Open globe valve

  Then make the following entries.

1. Enter the number of T-fittings that have one output flow and press <T->>.
2. Enter the number of T-fittings that have one input flow and press <->T>.
3. If you enter an incorrect number, enter the correct number and press the corresponding key.
4. Press <EOD> to proceed with the program.

(continued)

Specifying the Configuration (Continued)

After you enter the numbers of T fittings, the following display appears.

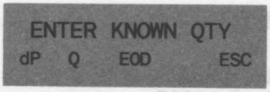
where the message displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨L⟩, INV ⟨U⟩, INV ⟨GTE⟩, or INV ⟨GLB⟩. To enter the pipe characteristics:

5. Enter the number of 90° elbow bends and press ⟨L⟩.
6. Enter the number of 180° elbow bends and press ⟨U⟩.
7. Enter the number of gate valves and press ⟨GTE⟩.
8. Enter the number of globe valves and press ⟨GLB⟩.
9. If you enter an incorrect number, enter the correct number and press the corresponding key.
10. Press ⟨EOD⟩ to proceed with the program.

Obtaining The Results

After you specify the configuration, the program prompts you to enter one of two quantities. It calculates the other quantity.



► To calculate Q:

1. Enter a value for the change in pressure in either pounds per in^2 (English) or kiloPascals (metric). Then press ⟨dP⟩.
2. Press ⟨EOD⟩.

The program displays the value of Q. English flow rate is expressed in gallons per minute and metric flow rate is in m^3 per minute.

► To calculate dP:

1. Enter a value for the flow rate in either gallons per minute (English) or m^3 per minute (metric). Then press ⟨Q⟩.
2. Press ⟨EOD⟩.

The program displays the value of dP. English pressure is expressed in pounds per in^2 and metric pressure is in kiloPascals.

You can enter several values for dP to see how the flow rate is affected, or you can enter several values for Q to see how the change in pressure is affected. You can also alternate between entries for dP and entries for Q.

Example: Estimating Pressure Drop

The following example illustrates how to use the Pipe Design for Liquid Flow program.

Example

A centrifugal pump takes brine from the bottom of a supply tank and delivers it into a higher discharge tank. The line between the tanks is Schedule–40, 6-inch pipe.

RHO = 73.63 lb/ft^3
MU = 2.9 lb/ft-hr
Inside Diameter = 0.5054 ft
Roughness (e) = 0.00015
Q = 810 gallons/minute
length = 700 ft
delta Z = 200 ft

There are two gate valves, four T-fittings that have one output flow, and four 90° elbow bends. Estimate the overall pressure drop (dP).

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨FLO⟩	LIQUID FLOW
Select English units	⟨ENG⟩	LIQUID FLOW
Enter the liquid flow	73.63 ⟨RHO⟩ 2.9 ⟨MU⟩ .5054 ⟨DIA⟩ ⟨EOD⟩	DIA = 0.5054
Enter the pipe characteristics	.00015 ⟨e⟩ 700 ⟨LEN⟩ 200 ⟨dZ⟩ ⟨EOD⟩	# OF FITTINGS
Specify the configuration	4 ⟨T–>⟩ ⟨EOD⟩ 4 ⟨L⟩ 2 ⟨GTE⟩ ⟨EOD⟩	ENTER KNOWN QTY
Obtain the result	810 ⟨Q⟩ ⟨EOD⟩	dP = 120.99

The discharge pressure is 120.99 lb/in^2 less than the supply pressure.

Chapter 8: Absorber Design

This chapter describes how to use the Absorber Design program, which uses the Edmister method to solve for the separations in a multicomponent absorption system.

Table of Contents

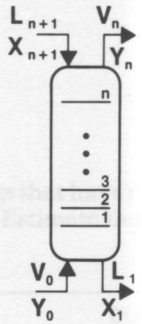
Absorber Design Introduction

The Absorber Design program assists in the design of absorbers by solving heat and material balances.

Design Method

The Absorber Design program uses the Edmister method to solve heat and material balances for multicomponent, multistage absorption. The method is a short-cut algorithm. As described in Treybal, the key to the method is assuming an effective absorption factor which is constant.

The Edmister method is based on an N-stage absorber with wet gas, V_0, fed to stage 1 and lean oil, L_{n+1}, fed to stage N. Leaving any stage n, the total liquid flow rate is L_n and the total vapor flow rate is V_n. Liquid and vapor flow rates of any component, i, leaving stage n are $L_n x_{in}$ and $V_n y_{in}$, where x is the mole fraction of component i in the liquid stream, and y is the mole fraction of component i in the vapor stream.



Initial Requirements

You must supply the number of trays, number of components, liquid and vapor temperature and molar flow rate, and an estimate of the tray efficiency. Next, for each component, you must enter liquid and vapor mole fractions, liquid and vapor molar heat capacities, latent heat of vaporization, and the K-value at the average operating temperature and pressure. Finally, you must provide an estimate of the individual component recovery factors.

Method of Calculation

This program calculates the effective absorption factor from the input data. It uses an iterative procedure to solve the heat and material balances at each stage, updating the component recovery factor and computing the liquid and gas compositions. When the program reaches a satisfactory approximation, it stops iterating and displays the recovery factor and the number of moles of each component in the exiting gas and liquid streams. Refer to Treybal for a detailed description of the Edmister method.

Reference

Treybal, R. E. 1972. *Mass-Transfer Operations*. 2nd ed. New York: McGraw-Hill.

The following procedure provides instructions for using the Absorber Design Program.

Before You Select the Program

Before you select this program, you need values for specific heat and latent heat of vaporization.

- If you do not have the value for specific heat, obtain it from the Specific Heat program (page 6–21) and convert it to the correct units before selecting this program.
- If you do not have the value for latent heat of vaporization, obtain it from the Latent Heat of Vaporization program (page 5–19) and convert it to the correct units before selecting this program.

Selecting the Program

To select the Absorber Design program:

1. Select ⟨DSN⟩ from the **CHEM ENGINEERING** menu. The program displays:

2. Select ⟨ABS⟩.

Defining the Absorber

After you select the program, the following display appears.

```
ABSORBER DESIGN
#Tr  #C   tlq  tvp  -->
```

Although the program does not prompt you to select English or metric units, you can enter data in either system.

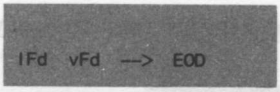
- For the program to generate results in English units, you enter all values expressed in English units.
- For the program to generate results in metric units, you enter all values expressed in metric units.

Refer to the entry procedures for the specific units.

You can check the current entries by pressing INV <#Tr>, INV <#C>, INV <tlq>, or INV <tvp>. To define the absorber:

1. Enter the number of trays in the absorber and press <#Tr>.
2. Enter the number of components feeding into the absorber and press <#C>.
3. Enter a value for the temperature of the entering liquid either in °F (English) or in °C (metric), and press <tlq>.
4. Enter a value for the temperature of the entering vapor either in °F (English) or in °C (metric), and press <tvp>.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press <-->> to display additional selections shown on the next page.

Defining the Absorber (Continued)



where the message displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨lFd⟩ or INV ⟨vFd⟩.

7. Enter the liquid feed rate in moles per time (the units of lFd and vFd must be the same), and press ⟨lFd⟩.

8. Enter the vapor feed rate in moles per time (the units of lFd and vFd must be the same), and press ⟨vFd⟩.

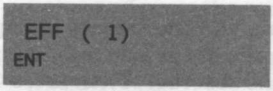
9. If you enter an incorrect value, enter the correct value and press the corresponding key.

10. If you want to return to the previous selections shown on the preceding page, press ⟨-->⟩.

11. Press ⟨EOD⟩ to proceed with the program.

Entering the Tray Efficiencies

After you define the absorber, the program displays:



You can check the current entry by pressing CE. To enter the efficiencies:

1. Enter a value for the efficiency of this tray and press ⟨ENT⟩.
2. Repeat step 1 for each tray.

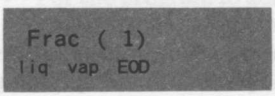
Editing the Tray Efficiencies

After you enter the last tray efficiency, the program displays:

- If you want to edit a value, press ⟨YES⟩ and go to Entering the Tray Efficiencies on the preceding page.
- If you do not want to edit any values, press ⟨NO⟩.

Entering the Material Fractions

After you select not to edit the tray efficiencies, the program displays:



You can check the current entries by pressing INV ⟨liq⟩ or INV ⟨vap⟩. To enter the material fractions:

1. Enter a value for the amount of liquid that is present in this component as a mole fraction of all the liquid entering the absorber. Then press ⟨liq⟩.

2. Enter a value for the amount of vapor that is present in this component as a mole fraction of all the vapor entering the absorber. Then press ⟨vap⟩.

3. If you enter an incorrect value, enter the correct value and press the corresponding key.

4. Press ⟨EOD⟩.

5. Repeat steps 1 through 4 for each component.

Because the total of all liquid mole fractions must be one and the total of all vapor mole fractions must be one, the program determines the last mole fractions without your entering them.

Entering the Component Properties

After the program determines the last mole fractions, the program displays:

```
COMPONENT  ( 1)
f    Cpl  Cpv  -->
```

You can check the current entries by pressing INV ⟨f⟩, INV ⟨Cpl⟩, or INV ⟨Cpv⟩. To enter the properties of a component:

1. Enter an estimate for the recovery factor of the component and press ⟨f⟩.

2. Enter a value for the specific heat of the component liquid either in BTU per pound mole °F (English) or in calories per gram mole °C (metric), and press ⟨Cpl⟩.

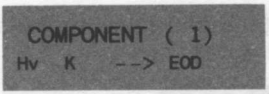
3. Enter a value for the specific heat of the component vapor either in BTU per pound mole °F (English) or in calories per gram mole °C (metric), and press ⟨Cpv⟩. The units for the liquid and vapor specific heat must be the same.

4. If you enter an incorrect value, enter the correct value and press the corresponding key.

5. Press ⟨-->⟩ to display additional selections shown on the next page.

(continued)

Entering the Component Properties (Continued)



You can check the current entries by pressing INV ⟨Hv⟩ or INV ⟨K⟩.

6. Enter a value for the heat of vaporization in BTU per pound mole (English) or in calories per gram mole (metric), and press ⟨Hv⟩.

7. Enter a value for the Depriester K-value and press ⟨K⟩.

8. If you enter an incorrect value, enter the correct value and press the corresponding key.

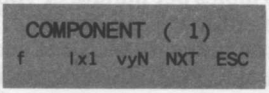
9. If you want to return to the previous selections shown on the preceding page, press ⟨-->⟩.

10. Press ⟨EOD⟩ to proceed with the program.

The program repeats the property entries for each component.

Obtaining the Results

After you enter the properties of the last component, the following display appears.



⟨f⟩ Displays a recovery factor for the component.

⟨lx1⟩ Displays the flow rate of liquid exiting the absorber in moles per time. The units of lx1 are the same as the units of vFd and lFd. (The meaning of this key symbol is "lx" for moles of liquid and "1" for tray 1.)

⟨vyN⟩ Displays the flow rate of vapor exiting the absorber in moles per time. The units of vyN are the same as the units of lFd and vFd. (The meaning of this key symbol is "vy" for moles of vapor and "N" for tray N.)

To obtain the results:

1. Press the keys that correspond to the results you want to view for this component.
2. Press ⟨NXT⟩ to advance to the next component.
3. Repeat steps 1 and 2 for each component.

Example: Estimating the Performance of an Absorber

The following example illustrates how to use the Absorber Design program.

Example

Estimate the performance of a three-tray, 100-percent-efficiency absorber, feeding 3.5 moles per minute of liquid and 1.0 moles per minute of vapor. Both the liquid and the vapor enter at 77 °F. Initially, a workable estimate for the recovery factor of each of the five components is 0.1. The following table gives the pertinent data for the components.

	Component Number				
	1	2	3	4	5
Liquid Fraction	0.00	0.00	0.00	0.01	0.99
Vapor Fraction	0.70	0.15	0.10	0.05	0.00
Cpl (BTU per pound mole °F)	0.00	25.10	27.80	33.10	90.00
Cpv (BTU per pound mole °F)	8.50	12.71	18.16	24.45	0.00
Hv (molal)	0	5100	7600	10100	0
K-value	50.00	13.50	4.25	1.25	0.10

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨ABS⟩	ABSORBER DESIGN
Define the absorber	3 ⟨#Tr⟩ 5 ⟨#C⟩ 77 ⟨tlq⟩ ⟨tvp⟩ ⟨-->⟩ 3.5 ⟨lFd⟩ 1 ⟨vFd⟩ ⟨EOD⟩	EFF(1)

Example (Continued)

Procedure	Press	Display
Enter the tray efficiencies	1 ⟨ENT⟩ 1 ⟨ENT⟩ 1 ⟨ENT⟩ ⟨NO⟩	EFF(2) EFF(3) Frac(1)
Enter the material fractions	0 ⟨liq⟩ .7 ⟨vap⟩ ⟨EOD⟩	Frac(2)
	0 ⟨liq⟩ .15 ⟨vap⟩ ⟨EOD⟩	Frac(3)
	0 ⟨liq⟩ .1 ⟨vap⟩ ⟨EOD⟩	Frac(4)
	.01 ⟨liq⟩ .05 ⟨vap⟩ ⟨EOD⟩	COMPONENT(1)
Enter the properties	.1 ⟨f⟩ 0 ⟨Cpl⟩ 8.5 ⟨Cpv⟩ ⟨-->⟩ 0 ⟨Hv⟩ 50 ⟨K⟩ ⟨EOD⟩	COMPONENT(2)
	.1 ⟨f⟩ 25.1 ⟨Cpl⟩ 12.71 ⟨Cpv⟩ ⟨-->⟩ 5100 ⟨Hv⟩ 13.5 ⟨K⟩ ⟨EOD⟩	COMPONENT(3)
	.1 ⟨f⟩ 27.8 ⟨Cpl⟩ 18.16 ⟨Cpv⟩ ⟨-->⟩ 7600 ⟨Hv⟩ 4.25 ⟨K⟩ ⟨EOD⟩	COMPONENT(4)
	.1 ⟨f⟩ 33.1 ⟨Cpl⟩ 24.45 ⟨Cpv⟩ ⟨-->⟩ 10100 ⟨Hv⟩ 1.25 ⟨K⟩ ⟨EOD⟩	COMPONENT(5)

(continued)

Example (Continued)

Procedure	Press	Display
Enter the properties of the last component	.1 ⟨f⟩ 90 ⟨Cpl⟩ 0 ⟨Cpv⟩ ⟨--->⟩ 0 ⟨Hv⟩ .1 ⟨K⟩ ⟨EOD⟩	COMPONENT(1)
View the results	⟨f⟩	f = .0818879877
	⟨lx1⟩	lx1 = .0573215914
	⟨vyN⟩	vyN = .6426784086
	⟨NXT⟩	COMPONENT(2)
	⟨f⟩	f = 0.301932818
	⟨lx1⟩	lx1 = .0452899227
	⟨vyN⟩	vyN = .1047100773
	⟨NXT⟩	COMPONENT(3)
	⟨f⟩	f = 0.748820961
	⟨lx1⟩	lx1 = .0748820961
	⟨vyN⟩	vyN = .0251179039
	⟨NXT⟩	COMPONENT(4)
	⟨f⟩	f = 0.982359388
	⟨lx1⟩	lx1 = 0.083500548
	⟨vyN⟩	vyN = 0.001499452
	⟨NXT⟩	COMPONENT(5)
	⟨f⟩	f = .9999879031
	⟨lx1⟩	lx1 = 3.464958084
	⟨vyN⟩	vyN = .0000419158

Chapter 9: Distillation Design

This chapter describes how to use the Distillation Design program, which uses the Fenske-Underwood-Gilliland Short-Cut Distillation Method to determine designs for distillation processes.

Table of Contents

Distillation Design Introduction

The Distillation Design program calculates the minimum number of ideal trays, the minimum reflux ratio, and the actual number of ideal trays for a multicomponent distillation column.

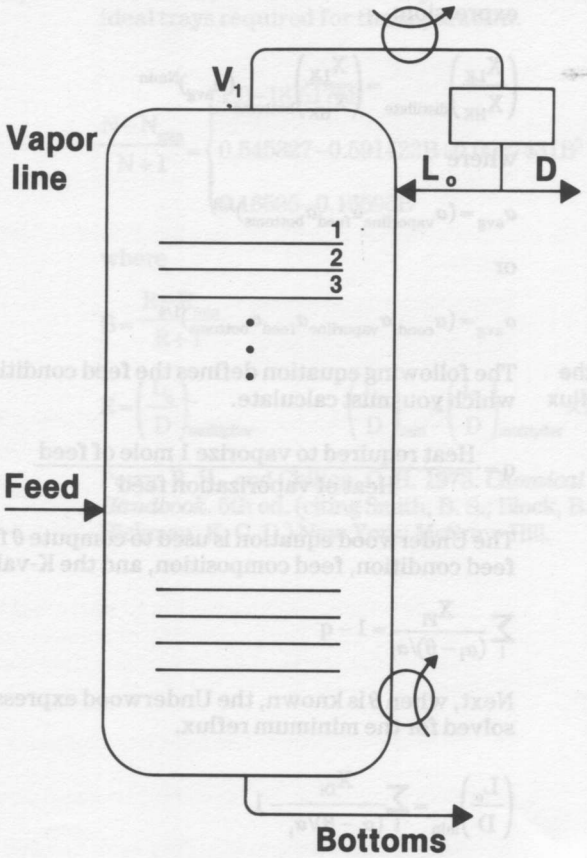
Design Methods

This program combines three short-cut methods in the preliminary design of a multicomponent distillation column. First, the Fenske method estimates the minimum number of trays required for the separation. Second, the Underwood method estimates the minimum reflux required in the column. Third, the Gilliland equation computes the actual number of trays as a function of the minimum and actual reflux ratios.

Initial Requirements

To use the program, first determine the composition of the feed stream, the distillate, and the bottoms. You must enter the K-values for the components at the column's average temperature and in order of their decreasing volatility. If the condenser is a total condenser, you must give the K-values of each component at the condenser temperature.

You also must choose one component to be the light key in the separation and one component to be the heavy key. The program requires that the key components be adjacent in volatility.


V_1
Vapor line
L_o
D
1
2
3
Feed
Bottoms

Calculating the Minimum Number of Ideal Trays

After you have designated the key components and entered the K-value data, the program calculates the minimum number of ideal trays from the Fenske expression:

$$\left(\frac{X_{LK}}{X_{HK}}\right)_{distillate} = \left(\frac{X_{LK}}{X_{HK}}\right)_{bottoms} (\alpha_{avg})^{Nmin}$$

where

$$\alpha_{avg} = (\alpha_{vaporline}\alpha_{feed}\alpha_{bottoms})^{1/3}$$

or

$$\alpha_{avg} = (\alpha_{cond.}\alpha_{vaporline}\alpha_{feed}\alpha_{bottoms})^{1/4}$$

Calculating the Minimum Reflux

The following equation defines the feed condition, q, which you must calculate.

$$q = \frac{\text{Heat required to vaporize 1 mole of feed}}{\text{Heat of vaporization feed}}$$

The Underwood equation is used to compute θ from the feed condition, feed composition, and the K-values.

$$\sum_i \frac{X_{Fi}}{(\alpha_i - \theta)/\alpha_i} = 1 - q$$

Next, when θ is known, the Underwood expression is solved for the minimum reflux.

$$\left(\frac{L_o}{D}\right)_{min} = \sum_i \frac{X_{Di}}{(\alpha_i - \theta)/\alpha_i} - 1$$

Calculating the Actual Number of Ideal Trays

Finally, the program determines the actual reflux by multiplying the L_o/D multiplier by the minimum reflux. The Gilliland correlation computes the actual number of ideal trays required for the separation.

$$\frac{N-N_{min}}{N+1}=\begin{cases}1.0-18.5175B & 0\leq B\leq 0.01\\ 0.545827-0.591422B+0.0027431B^2 & 0.01<B\leq 0.9\\ 0.16595-0.16595B & 0.9<B\leq 1\end{cases}$$

where

$$B=\frac{R-R_{min}}{R+1}$$

$$R=\left(\frac{L_o}{D}\right)_{multiplier} \qquad \left(\frac{L_o}{D}\right)_{min}=\left(\frac{L_o}{D}\right)_{multiplier}\times R_{min}$$

Reference

Perry, R. H., and Chilton, C. H. 1973. *Chemical Engineers' Handbook*. 5th ed. (citing Smith, B. S.; Block, B.; and Hickman, K. C. D.) New York: McGraw-Hill.

The following procedure provides instructions for using the Distillation Design program.

Selecting the Program

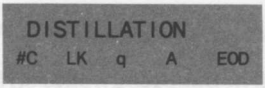
To select the Distillation Design program:

1. Select ⟨DSN⟩ from the **CHEM ENGINEERING** menu. The program displays:

2. Select ⟨DIS⟩.

Defining the Distillation Process

After you select the program, the following display appears.



You can check the current entries by pressing INV ⟨#C⟩, INV ⟨LK⟩, INV ⟨q⟩, or INV ⟨A⟩. To define the distillation process:

1. Enter the number of components in the mixture and press ⟨#C⟩.
2. Decide which components are to be the light key and the heavy key. The numbering of components must be such that the light key is one less than the heavy key.
3. Enter the number of the light key and press ⟨LK⟩.
4. Enter a value for the feed condition and press ⟨q⟩.
5. Enter a value for actual reflux ratio divided by the minimum reflux ratio $(L_o/D)_{min}$ and press ⟨A⟩.
6. If you enter an incorrect value, enter the correct value and press the corresponding key.
7. Press ⟨EOD⟩ to proceed with the program.

Entering the K-Values for the Light Key

After you define the distillation process, the program displays:

```
K-LIGHT KEY
Fd   Vap  Bot  EOD
```

You can check the current entries by pressing INV ⟨Fd⟩, INV ⟨Vap⟩, or INV ⟨Bot⟩. To enter the K-values for the light key:

1. Enter a value for K at the feed mixture and press ⟨Fd⟩.
2. Enter a value for K at the vapor line and press ⟨Vap⟩.
3. Enter a value for K at the bottoms and press ⟨Bot⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Entering the K-Values for the Heavy Key

After you enter the K-values for the light key, the program displays:

```
K-HEAVY KEY
Fd   Vap  Bot  EOD
```

You can check the current entries by pressing [INV] ⟨Fd⟩, [INV] ⟨Vap⟩, or [INV] ⟨Bot⟩. To enter the K-values for the heavy key:

1. Enter a value for K at the feed mixture and press ⟨Fd⟩.
2. Enter a value for K at the vapor line and press ⟨Vap⟩.
3. Enter a value for K at the bottoms and press ⟨Bot⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Entering the Condenser K-Values

After you enter the K-values for the heavy key, the following display appears.

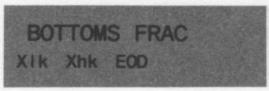
You can check the current entries by pressing INV ⟨Klk⟩ or INV ⟨Khk⟩.

- If there is no condenser, press ⟨NIL⟩ ⟨EOD⟩ and go to the next page.
- If there is a condenser:

  1. Enter a value for K of the light key in the condenser and press ⟨Klk⟩.
  2. Enter a value for K of the heavy key in the condenser and press ⟨Khk⟩.
  3. If you enter an incorrect value, enter the correct value and press the corresponding key.
  4. Press ⟨EOD⟩ to proceed with the program.

Entering the Key Fractions of the Bottoms

After you enter the condenser K-values or you indicate there is no condenser, the program displays:



You can check the current entries by pressing INV ⟨Xlk⟩ or INV ⟨Xhk⟩. To enter the key fractions of the bottoms:

1. Determine the composition of the mixture in the bottoms. The mixture may consist of the light key, the heavy key, and other components.
2. Enter a value for the mole fraction of the light key and press ⟨Xlk⟩.
3. Enter a value for the mole fraction of the heavy key and press ⟨Xhk⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

Entering the Data for the Components

After you enter the key fractions of the bottoms, the program displays:

You can check the current entries by pressing INV ⟨K⟩, INV ⟨Xfd⟩, or INV ⟨Xdi⟩. To enter data for this component:

1. Enter a value for K of the component at the average temperature of the distillation system and press ⟨K⟩.

2. Enter the mole fraction of the component in the feed mixture and press ⟨Xfd⟩.

3. Enter the mole fraction of the component in the distillate and press ⟨Xdi⟩.

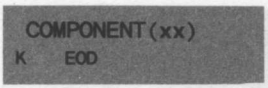
4. If you enter an incorrect value, enter the correct value and press the corresponding key.

5. Press ⟨EOD⟩ to proceed with the program.

The program prompts you to enter the data for each component until all but the last component are entered.

Entering the Data for the Last Component

After you enter the data for all but the last component, the program displays:



where xx is the number of the last component.

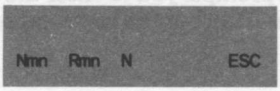
You can check the current entry by pressing INV ⟨K⟩. To enter data for the last component:

1. Enter a value for K of the last component at the average temperature of the distillation system and press ⟨K⟩.
2. If you enter an incorrect value, enter the correct value and press ⟨K⟩.
3. Press ⟨EOD⟩ to proceed with the program.

Because the total of all mole fractions in the feed must be one and the total of all mole fractions in the distillate must be one, the program determines the last mole fractions without your entering them.

Obtaining the Results

After you enter the last component, the following display appears.



where the value displayed when this menu first appears is the last value generated (N).

⟨Nmn⟩ Displays the minimum number of trays required at infinite reflux.

⟨Rmn⟩ Displays a value for the minimum reflux ratio.

⟨N⟩ Displays the number of trays required for the actual reflux ratio.

View each result that you want to see by pressing the key that corresponds to that result.

Example: Estimating the Number of Trays

The following example illustrates how to use the Distillation Design program.

Example

Estimate the actual number of ideal trays required to perform the separation of a seven-component system corresponding to the data given below.

The feed is a saturated vapor (feed condition, q, is 0). The L_o/D multiplier, A, is 1.3. No condenser is present.

	K-value in Feed	K-value in Distillate	K-value in Bottoms	Mole Fraction in Bottoms
Light key (Component 3)	4.2	0.54	2.7	0.028
Heavy key (Component 4)	3.5	0.35	2.1	0.292

Component	K-value at Average Temperature	Feed Mole Fraction	Distillate Mole Fraction
1	18.0	0.060	0.214
2	8.0	0.120	0.429
3 (light key)	4.2	0.110	0.321
4 (heavy key)	3.5	0.220	0.036
5	2.4	0.060	0.000
6	1.4	0.180	0.000
7	0.32	0.250	0.000

Example (Continued)

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨DIS⟩	DISTILLATION
Define the process	7 ⟨#C⟩ 3 ⟨LK⟩ 0 ⟨q⟩ 1.3 ⟨A⟩ ⟨EOD⟩	K-LIGHT KEY
Enter K-values for the light key	4.2 ⟨Fd⟩ .54 ⟨Vap⟩ 2.7 ⟨Bot⟩ ⟨EOD⟩	K-HEAVY KEY
Enter K-values for the heavy key	3.5 ⟨Fd⟩ .35 ⟨Vap⟩ 2.1 ⟨Bot⟩ ⟨EOD⟩	K-CONDENSER
Select no condenser	⟨NIL⟩ ⟨EOD⟩	BOTTOMS FRAC
Enter key fractions for the bottoms	.028 ⟨Xlk⟩ .292 ⟨Xhk⟩ ⟨EOD⟩	COMPONENT(1)

Example (Continued)

Procedure	Press	Display
Enter data for the components	18 ⟨K⟩ .06 ⟨Xfd⟩ .214 ⟨Xdi⟩ ⟨EOD⟩	COMPONENT(2)
	8 ⟨K⟩ .12 ⟨Xfd⟩ .429 ⟨Xdi⟩ ⟨EOD⟩	COMPONENT(3)
	4.2 ⟨K⟩ .11 ⟨Xfd⟩ .321 ⟨Xdi⟩ ⟨EOD⟩	COMPONENT(4)
	3.5 ⟨K⟩ .22 ⟨Xfd⟩ .036 ⟨Xdi⟩ ⟨EOD⟩	COMPONENT(5)
	2.4 ⟨K⟩ .06 ⟨Xfd⟩ 0 ⟨Xdi⟩ ⟨EOD⟩	COMPONENT(6)
	1.4 ⟨K⟩ .18 ⟨Xfd⟩ 0 ⟨Xdi⟩ ⟨EOD⟩	COMPONENT(7)
Enter the last K-value	.32 ⟨K⟩ ⟨EOD⟩	28.58
View the results	⟨Nmn⟩	Nmn = 15.68
	⟨Rmn⟩	Rmn = 6.91
	⟨N⟩	N = 28.58

Chapter 10: Heat Exchanger Design

This chapter describes how to use the Heat Exchanger Design program which determines the sizing of double-pipe or shell and tube heat exchangers.

Table of Contents

Heat Exchanger Design Introduction

The Heat Exchanger Design program uses a modified Kern method to design shell and tube heat exchangers. You may use this program in conjunction with programs such as Liquid Viscosity, Specific Heat, Pipe Design for Liquid Flow, and Heat Transfer Coefficient Estimation.

Log Mean Temperature Difference Option (MdT)

The program estimates the log mean temperature difference from the hot and cold incoming stream temperatures and your choice of combinations of outgoing stream temperatures, flow rates, heat capacities, and heat transfer rate.

Depending on the temperatures supplied, the program checks the heat balance relationship

$$\dot{m}_h C_{Ph}(T_i - T_o) = \dot{m}_c C_{Pc}(t_o - t_i)$$

and supplies the missing temperature, if necessary.

The program then calculates the log mean temperature difference

$$\Delta T_{lm} = LMTD = \frac{(T_i - t_o) - (T_o - t_i)}{\ln((T_i - t_o)/(T_o - t_i))}$$

and the MdT correction factor for both a one-shell pass/two-tube pass exchanger and a two-shell pass/four-tube pass exchanger.

Geometry Option

The program estimates the overall heat transfer coefficient from the internal and external heat transfer coefficients, the heat transfer rate, the log mean temperature difference, and the dirt factor (see Kern).

$$U_o = \frac{(h_i)_o (h_o)_o}{(h_i)_o + (h_o)_o}$$

When you supply the heat exchanger duty, the program calculates the required heat transfer area.

$$A = \frac{Q}{U_o \Delta T_{lm} F_t}$$

The number of tubes in the exchanger is computed from the tube diameter, the surface area required, and the tube length.

Pressure Drop Option

The program estimates pressure drop on the shell side of the heat exchanger from the flow rate, viscosity, and density of the fluid in the shell side. The calculation also requires the heat exchanger dimensions.

The pressure drop on the shell side is estimated from the equation

$$\Delta P = (1.52)(10^{-10})\left(\frac{\omega}{S_p}\right)^{1.808}\left(\frac{L}{ID^{0.808}B^{2.808}}\right)\left[\frac{1}{D_e^{1.192}}\left(\frac{P_T}{P_T - d_o}\right)^{1.808}\right]\left(\frac{\mu^{0.192}}{S}\right)$$

where

	English Units	Metric Units
S_P = No. of Shell Passes		
w = Shell-side Flow Rate	lb/hr	Kg/hr
ID = Shell Inside Diameter	inches	m
B = Baffle Spacing	inches	m
L = Length of Tubes	inches	m
d_o = Tube Outside Diameter	inches	m
D_e = Shell Equivalent Diameter	ft	m
P_T = Tube Pitch	inches	m
μ = Fluid Viscosity	lb/ft-hr	centipoise
s = Fluid Specific Gravity		

D_e is defined as

$$D_e = \frac{0.0835(1.27P_T^2 - d_o^2)}{d_o} \qquad \text{Square Pitch}$$

$$D_e = \frac{0.0835(1.11P_T^2 - d_o^2)}{d_o} \qquad \text{Triangular Pitch}$$

Pressure Drop Option (Continued)

The program estimates pressure drop on the tube side of the heat exchanger from the flow rate, viscosity, and specific gravity of the fluid in the tube side. The calculation also requires the heat exchanger dimensions and tube roughness.

The pressure drop on the tube side is estimated from the equation

$$\Delta P_T = \Delta P_t + \Delta P_r$$

The ΔP_t term represents the pressure drop due to flow in the tubes. It is calculated from

$$\Delta P_t = \frac{f \omega L n}{5.22 \times 10^{10} (ID_t)(S)(a_t^2)}$$

where

$a_t' =$ Flow Area/Tube [in^2]

$N_t =$ Number of Tubes

$n =$ Number of Tube Passes

$$a_t = \frac{N_t a_t'}{144n}$$

$$f = \text{Friction Factor} = 0.035 + (0.264)\left(\frac{a_t \mu}{ID_t \omega}\right)^{0.42}$$

The ΔP_r term comes from losses due to expansion and contraction of the fluid flow, where

$$\Delta P_r = \frac{0.02696n}{S}\left(\frac{\omega}{a_t p(3600)}\right)^2$$

Note: Because of the dimensional nature of the equations in the geometry portion of the program, the values you enter for variables must be in the units specified.

Reference

Kern, D. Q. 1950. *Process Heat Transfer*. New York: Addison-Wesley.

The Heat Exchanger Design Program

The following procedure provides instructions for using the Heat Exchanger Design program.

Before You Select the Program

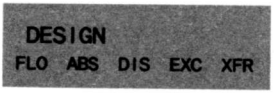
Before you select this program, you need the value for specific heat and possibly values for viscosity and density.

- If you do not have the value for specific heat, obtain it from the Specific Heat program (page 6–21) before running this program.
- If you are analyzing an exchanger from the dimensions in contact with fluid in the shell and you do not have the values for viscosity and density, obtain them from the viscosity and density programs (pages 4–2 and 4–26) before running this program.

Selecting the Program

To select the Heat Exchanger Design program:

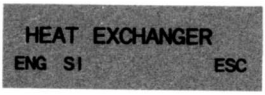
1. Select ⟨DSN⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨EXC⟩.

Selecting the Units

After you select the program, the following display appears.



- If your entries and results are to be in the English system of units, press ⟨ENG⟩.
- If your entries and results are to be in the metric (SI, System International) system of units, press ⟨SI⟩.

If you run the program with one set of units and then return to this display and select the other set of units, the numbers you entered previously are converted automatically.

Selecting a Calcuation Option

After you select the units, the program displays:

```
HEAT EXCHANGER
MdT  GEO  dP        ESC
```

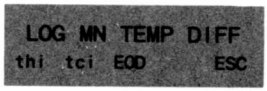
- To calculate the log of mean temperature difference, press ⟨MdT⟩. The instructions for this option begin on the next page.
- To calculate the exchanger geometry, press ⟨GEO⟩. Go to page 10–19 for the instructions for this option.
- To calculate the pressure drop, press ⟨dP⟩. Go to page 10–23 for the instructions for this option.

The Log Mean dT Calculation Option

The following procedure provides instructions for using the log mean temperature difference calculation option of the Heat Exchanger Design program.

Entering the Incoming Temperatures

When you select the log mean temperature difference calculation option, the program displays:



You can check the current entries by pressing INV ⟨thi⟩ or INV ⟨tci⟩. To enter the incoming fluid stream temperatures:

1. Enter a value for the incoming hot fluid temperature in either °F (English) or °C (metric). Then press ⟨thi⟩.
2. Enter a value for the incoming cold fluid temperature in either °F (English) or °C (metric). Then press ⟨tci⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.

Specifying the Entry Sequence

After you enter the incoming temperatures, the program displays:

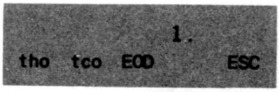
```
KNOWN EXIT QTYS
2t  thQ th  tcQ tc
```

You can choose which quantities pertaining to the outgoing fluid stream to supply to the program. Use the following table to decide which entry sequence to select.

If You Know	Press	Go to Page
Both outgoing fluid temperatures	⟨2t⟩	10–9
Hot fluid outgoing temperature Quantity of heat transferred per time Cold fluid specific heat Cold fluid flow rate	⟨thQ⟩	10–10
Hot fluid outgoing temperature Hot fluid specific heat Cold fluid specific heat Hot fluid flow rate Cold fluid flow rate	⟨th⟩	10–12
Cold fluid outgoing temperature Quantity of heat transferred per time Hot fluid specific heat Hot fluid flow rate	⟨tcQ⟩	10–14
Cold fluid outgoing temperature Hot fluid specific heat Cold fluid specific heat Hot fluid flow rate Cold fluid flow rate	⟨tc⟩	10–16

Entering Both Outgoing Temperatures

If you specify the option for which both outgoing temperatures are known, the program displays:



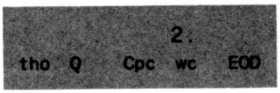
You can check the current entries by pressing [INV] ⟨tho⟩ or [INV] ⟨tco⟩. To enter the outgoing fluid stream temperatures:

1. Enter a value for the outgoing hot fluid temperature in either °F (English) or °C (metric). Then press ⟨tho⟩.
2. Enter a value for the outgoing cold fluid temperature in either °F (English) or °C (metric). Then press ⟨tco⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.

The program calculates the results, described on page 10–18.

Entering the Hot Outgoing Temperature and Heat Quantity

If you specify the option for which the hot fluid outgoing temperature and the quantity of heat transferred are known, the program displays:

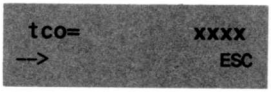


You can check the current entries by pressing INV ⟨tho⟩, INV ⟨Q⟩, INV ⟨Cpc⟩, or INV ⟨wc⟩. To enter the data:

1. Enter a value for the outgoing hot fluid temperature in either °F (English) or °C (metric). Then press ⟨tho⟩.
2. Enter a value for the heat transfer rate in either BTU per hour (English) or Watts (metric). Then press ⟨Q⟩.
3. Enter a value for the cold fluid specific heat in either BTU per pound °F (English) or calories per gram °C (metric). Then press ⟨Cpc⟩.
4. Enter a value for the cold fluid flow rate in either pounds per hour (English) or kilograms per hour (metric). Then press ⟨wc⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ to proceed with the program.

Viewing the Missing Temperature

After you enter the data, the program calculates the cold fluid outgoing temperature.

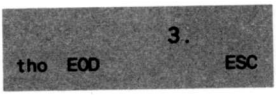


where xxxx is this temperature in °F (English) or °C (metric).

To proceed with the program, press ⟨-->⟩. The program then calculates the results, described on page 10–18.

Entering the Hot Outgoing Temperature

If you specify the option for which the hot fluid outgoing temperature is known, the program displays:



You can check the current entry by pressing INV ⟨tho⟩. To enter the outgoing hot fluid stream temperature:

1. Enter a value for the outgoing hot fluid temperature in either °F (English) or °C (metric). Then press ⟨tho⟩.
2. If you enter an incorrect value, enter the correct value and press ⟨tho⟩.
3. Press ⟨EOD⟩ to proceed with the program.

Entering the Hot Outgoing Temperature (Continued)

```
 tho=              xxxx
Cph  wh   Cpc  wc   EOD
```

where xxxx is this temperature in °F (English) or °C (metric).

You can check the current entries by pressing INV ⟨Cph⟩, INV ⟨wh⟩, INV ⟨Cpc⟩, or INV ⟨wc⟩. To continue entering the data:

4. Enter a value for the hot fluid specific heat in either BTU per pound °F (English) or calories per gram °C (metric). Then press ⟨Cph⟩.

5. Enter a value for the hot fluid flow rate in either pounds per hour (English) or kilograms per hour (metric). Then press ⟨wh⟩.

6. Enter a value for the cold fluid specific heat in either BTU per pound °F (English) or calories per gram °C (metric). Then press ⟨Cpc⟩.

7. Enter a value for the cold fluid flow rate in either pounds per hour (English) or kilograms per hour (metric). Then press ⟨wc⟩.

8. If you enter an incorrect value, enter the correct value and press the corresponding key.

9. Press ⟨EOD⟩ to proceed with the program.

Viewing the Missing Temperature

The program calculates the cold fluid outgoing temperature.

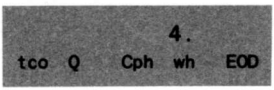
```
 tco=              xxxx
-->
```

where xxxx is this temperature in °F (English) or °C (metric).

To proceed with the program, press ⟨-->⟩. The program calculates the results, described on page 10–18.

Entering the Cold Outgoing Temperature and Heat Quantity

If you specify the option for which the cold fluid outgoing temperature and the quantity of heat transferred are known, the program displays:



You can check the current entries by pressing INV ⟨tco⟩, INV ⟨Q⟩, INV ⟨Cph⟩, or INV ⟨wh⟩. To enter the data:

1. Enter a value for the outgoing cold fluid temperature in either °F (English) or °C (metric). Then press ⟨tco⟩.
2. Enter a value for the heat transfer rate in either BTU per hour (English) or Watts (metric). Then press ⟨Q⟩.
3. Enter a value for the hot fluid specific heat in either BTU per pound °F (English) or calories per gram °C (metric). Then press ⟨Cph⟩.
4. Enter a value for the hot fluid flow rate in either pounds per hour (English) or kilograms per hour (metric). Then press ⟨wh⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ to proceed with the program.

Viewing the Missing Temperature

The program calculates the hot fluid outgoing temperature.

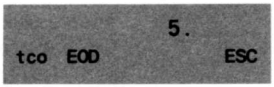
```
 tho=              xxxx
-->
```

where xxxx is this temperature in °F (English) or °C (metric).

To proceed with the program, press <-->. The program calculates the results, described on page 10–18.

Entering the Cold Outgoing Temperature

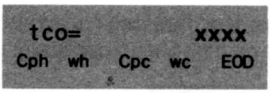
If you specify the option for which the cold fluid outgoing temperature is known, the program displays:



You can check the current entry by pressing INV ⟨tco⟩. To enter the outgoing cold fluid stream temperature:

1. Enter a value for the outgoing cold fluid temperature in either °F (English) or °C (metric). Then press ⟨tco⟩.
2. If you enter an incorrect value, enter the correct value and press ⟨tco⟩.
3. Press ⟨EOD⟩ to proceed with the program.

Entering the Cold Outgoing Temperature (Continued)



where xxxx is this temperature in °F (English) or °C (metric).

You can check the current entries by pressing INV ⟨Cph⟩, INV ⟨wh⟩, INV ⟨Cpc⟩, or INV ⟨wc⟩. To continue entering the data:

4. Enter a value for the hot fluid specific heat in either BTU per pound °F (English) or calories per gram °C (metric). Then press ⟨Cph⟩.

5. Enter a value for the hot fluid flow rate in either pounds per hour (English) or kilograms per hour (metric). Then press ⟨wh⟩.

6. Enter a value for the cold fluid specific heat in either BTU per pound °F (English) or calories per gram °C (metric). Then press ⟨Cpc⟩.

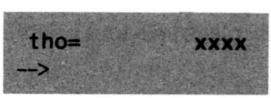
7. Enter a value for the cold fluid flow rate in either pounds per hour (English) or kilograms per hour (metric). Then press ⟨wc⟩.

8. If you enter an incorrect value, enter the correct value and press the corresponding key.

9. Press ⟨EOD⟩ to proceed with the program.

Viewing the Missing Temperature

The program calculates the hot fluid outgoing temperature.

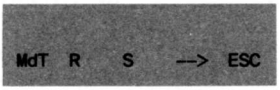


where xxxx is this temperature in °F (English) or °C (metric).

To proceed with the program, press ⟨-->⟩. The program calculates the results, described on the next page.

Obtaining the Results

After you enter the data and the program calculates any missing temperature, the program displays:



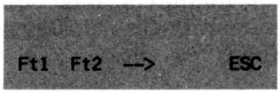
where the number displayed is the last value generated (Ft2) or left over from the previous menu.

〈MdT〉 Displays the log of the mean temperature difference. English temperature difference is expressed in °F and metric temperature difference in °C.

〈R〉 Displays the value of R for finding values of Ft in an Ft table.

〈S〉 Displays the value of S for finding values of Ft in an Ft table.

〈-->〉 Displays additional selections shown below.



where the value displayed when you select this menu is left over from the previous menu.

〈Ft1〉 Displays the value of Ft for a 1–2 heat exchanger configuration.

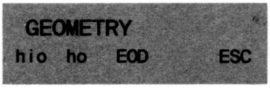
〈Ft2〉 Displays the value of Ft for a 2–4 heat exchanger configuration.

〈-->〉 Displays previous selections shown above.

The following procedure provides instructions for using the geometry calculation option of the Heat Exchanger Design program.

Entering the Heat Transfer Coefficients

When you select the geometry calculation option, the program displays:



You can check the current entries by pressing [INV] ⟨hio⟩ or [INV] ⟨ho⟩. To enter the heat transfer coefficients:

1. Enter the inside (tube side) initial heat transfer coefficient in either BTU per hour-foot^2-°F (English) or Watts per meter^2-°C (metric). Then press ⟨hio⟩.

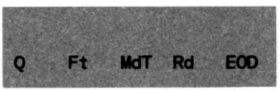
2. Enter the outside (shell side) initial heat transfer coefficient in either BTU per hour-foot^2-°F (English) or Watts per meter^2-°C (metric). Then press ⟨ho⟩.

3. If you enter an incorrect value, enter the correct value and press the corresponding key.

4. Press ⟨EOD⟩ to proceed with the program.

Entering the Heat Exchanger Parameters

After you enter the heat transfer coefficients, the program displays:



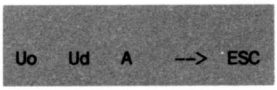
where the value displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨Q⟩, INV ⟨Ft⟩, INV ⟨Mdt⟩, or INV ⟨Rd⟩. To enter the heat exchanger parameters:

1. Enter a value for the heat transfer rate in either BTU per hour (English) or Watts (metric). Then press ⟨Q⟩.
2. Enter a value for the heat exchanger configuration and press ⟨Ft⟩.
3. Enter a value for the log of the mean temperature difference in either °F (English) or °C (metric). Then press ⟨MdT⟩.
4. Enter a value for the dirt factor in either hour-foot^2-°F per BTU (English) or meter^2-°C per Watt (metric). Then press ⟨Rd⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ to proceed with the program.

Reviewing the Basic Design

After you enter the heat exchanger parameters, the program displays:



where the value displayed when this menu first appears is left over from the previous menu.

⟨Uo⟩ Displays the value for the overall design coefficient in either BTU per hour-foot^2-°F (English) or Watts per meter^2-°C (metric).

⟨Ud⟩ Displays the value for the dirt-compensated design coefficient in either BTU per hour-foot^2-°F (English) or Watts per meter^2-°C (metric).

⟨A⟩ Displays the value for the area in either square feet (English) or square meters (metric).

To review the design:

1. View each quantity that you want to see by pressing the key that corresponds to that quantity.

2. Press ⟨-->⟩ to proceed with the program.

Calculating the Number of Tubes

After you review the basic design, the program displays:

```
CALC # TUBES
LEN DIA EOD      ESC
```

You can check the current entries by pressing [INV] ⟨LEN⟩ or [INV] ⟨DIA⟩. To calculate the number of tubes:

1. Enter a value for the length of the heat exchanger in either feet (English) or meters (metric). Then press ⟨LEN⟩.
2. Enter a value for the tube diameter in either feet (English) or meters (metric). Then press ⟨DIA⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ and the program displays:

```
# TUBES=     xxxx
                ESC
```

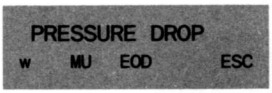
where xxxx is the number of tubes.

The Pressure Drop Calculation Option

The following procedure provides instructions for using the pressure drop calculation option of the Heat Exchanger Design program.

Entering the External Conditions

When you select the pressure drop calculation option, the program displays:



You can check the current entries by pressing INV ⟨w⟩ or INV ⟨MU⟩. To enter the external conditions:

1. Enter a value for the flow rate of either the fluid in contact with the shell or the fluid in the tubes, depending on the design option you select. The units are either pounds per hour (English) or kilograms per hour (metric). Then press ⟨w⟩.

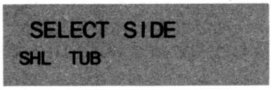
2. Enter a value for the viscosity of the liquid in either lb/ft-hr (English) or centipoise (metric). Then press ⟨MU⟩.

3. If you enter an incorrect value, enter the correct value and press the corresponding key.

4. Press ⟨EOD⟩ to proceed with the program.

Selecting a Design Option

After you enter the external conditions, the program displays:

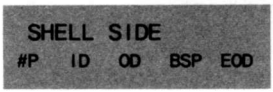


- If you know the dimensions in contact with the fluid in the shell, press ⟨SHL⟩. This entry sequence is described on the next page.

- If you know the dimensions in contact with the fluid in the tubes, press ⟨TUB⟩. This entry sequence is described on page 10–27.

Entering the Exchanger Dimensions

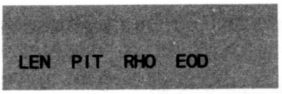
If you specify the option for which the dimensions in contact with the fluid in the shell are known, the program displays:



You can check the current entries by pressing INV ⟨#P⟩, INV ⟨ID⟩, INV ⟨OD⟩, or INV ⟨BSP⟩. To enter the exchanger dimensions:

1. Enter the number of passes made by the shell in the length of the heat exchanger and press ⟨#P⟩.
2. Enter a value for the shell inside diameter. The units are inches (English) or meters (metric). Then press ⟨ID⟩.
3. Enter a value for the tube outside diameter. The units are inches (English) or meters (metric). Then press ⟨OD⟩.
4. Enter a value for the baffle spacing. The units are inches (English) or meters (metric). Then press ⟨BSP⟩.
5. If you enter an incorrect value, enter the correct value and press the corresponding key.
6. Press ⟨EOD⟩ to proceed with the program.

Entering the Exchanger Dimensions (Continued)



where the value displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨LEN⟩, INV ⟨PIT⟩, or INV ⟨RHO⟩. To continue entering the exchanger dimensions:

7. Enter a value for the length of the exchanger in either inches (English) or meters (metric). Then press ⟨LEN⟩.

8. Enter a value for the pitch of the tube centers in either inches (English) or meters (metric). Then press ⟨PIT⟩.

9. Enter a value for the density of the fluid in the shell in either lb/ft^3 (English) or g/cm^3 (metric). Then press ⟨RHO⟩.

10. If you enter an incorrect value, enter the correct value and press the corresponding key.

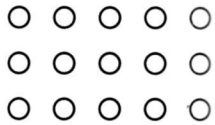
11. Press ⟨EOD⟩ to proceed with the program.

Specifying the Arrangement of Tubes

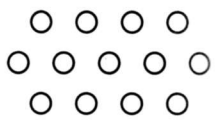
After you enter the exchanger dimensions, the program displays:

```
SELECT PITCH
SQR  TRI          ESC
```

- If the tubes are arranged with their centers on a square grid (depicted at right), press ⟨SQR⟩. Square-pitched tubes occupy planes that intersect at 90°.



- If the tubes are arranged with their centers on a triangular grid (depicited at right), press ⟨TRI⟩. Triangular pitched tubes occupy planes that intersect at 60°.



Obtaining the Result

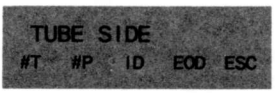
After you specify the arrangement of tubes, the program displays:

```
dP=              xxxx
                 ESC
```

where **xxxx** is this pressure drop expressed in lb/in^2.

Entering the Tube Data

When you specify the option for which the dimensions in contact with the fluid in the tube are known, the program displays:

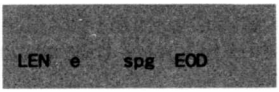


You can check the current entries by pressing INV ⟨#T⟩, INV ⟨#P⟩, or INV ⟨ID⟩. To enter the tube data:

1. Enter the number of tubes that connect directly to the fluid source and press ⟨#T⟩.
2. Enter the number of passes made by any single tube in the length of the heat exchanger and press ⟨#P⟩.
3. Enter a value for the tube inside diameter in either inches (English) or meters (metric). Then press ⟨ID⟩.
4. If you enter an incorrect value, enter the correct value and press the corresponding key.
5. Press ⟨EOD⟩ to proceed with the program.

(continued)

Entering the Tube Data (Continued)



where the value displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨LEN⟩, INV ⟨e⟩, or INV ⟨spg⟩. To continue entering the tube data:

6. Enter a value for the length of the exchanger in either inches (English) or meters (metric). Then press ⟨LEN⟩.

7. Enter a value for the roughness in either feet (English) or meters (metric). Then press ⟨e⟩.

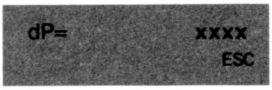
8. Enter a value for the specific gravity and press ⟨spg⟩.

9. If you enter an incorrect value, enter the correct value and press the corresponding key.

10. Press ⟨EOD⟩ to proceed with the program.

Viewing the Result

After you enter the tube data, the program displays:



where xxxx is this pressure drop expressed in lb/in^2.

Example 1: Calculating Exchanger Size, 2t Option

The following example illustrates how to use the Heat Exchanger Design program to calculate sizing.

Example

Determine the area required and the number of tubes for an exchanger that has the following requirements:

Hot fluid inlet temperature = 390 °F
Cold fluid inlet temperature = 100 °F
Hot fluid outlet temperature = 200 °F
Cold fluid outlet temperature = 170 °F
Inside heat transfer coefficient = 169 BTU/ft^2-hr-°F
Outside heat transfer coefficient = 109 BTU/ft^2-hr-°F
Hot fluid flow rate = 43800 lb/hr
Hot fluid Cp = 0.605 BTU/lb °F
Q = (43800 lb/hr) (0.605 BTU/lb °F) (390 °F–200 °F)
= 5,034,810 BTU/hr
Dirt factor (Rd) = 0.00348 ft^2-hr-°F/BTU

The tubes are 16 feet (192 inches) long and 0.75 inches in diameter.

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨EXC⟩	HEAT EXCHANGER
Select English units	⟨ENG⟩	HEAT EXCHANGER
Select log mean temperature difference	⟨MdT⟩	LOG MN TEMP DIFF
Enter incoming temperatures	390 ⟨thi⟩ 100 ⟨tci⟩ ⟨EOD⟩	KNOWN EXIT QTYS

(continued)

Example (Continued)

Procedure	Press		Display
Indicate that both outgoing temperatures are known	⟨2t⟩		1.
Enter outgoing temperatures	200 ⟨tho⟩ 170 ⟨tco⟩ ⟨EOD⟩		0.975
View the results	⟨MdT⟩	MdT =	152.2
	⟨R⟩	R =	2.714
	⟨S⟩	S =	0.241
	⟨-->⟩ ⟨Ft1⟩	Ft1 =	0.892
	⟨Ft2⟩	Ft2 =	0.975
Select geometry	⟨ESC⟩ ⟨ESC⟩ ⟨GEO⟩	GEOMETRY	
Enter the heat transfer coefficients	169 ⟨hio⟩ 109 ⟨ho⟩ ⟨EOD⟩	ho =	109.
Enter Q and the dirt factor	5034810 ⟨Q⟩ .00348 ⟨Rd⟩	Rd =	0.00348
Accept the entries for Ft and MdT	⟨EOD⟩		0.
View the design factors of the heat exchanger	⟨Uo⟩	Uo =	66.2626
	⟨Ud⟩	Ud =	53.846
	⟨A⟩	A =	688.7314
Calculate the number of tubes	⟨-->⟩ 16 ⟨LEN⟩ .0625 ⟨DIA⟩ ⟨EOD⟩	# TUBES =	219.23

Example 2: Calculating Exchanger Size, th Option

The following example illustrates how to use the Heat Exchanger Design program to calculate sizing.

Example

Specify the area required and the number of tubes for an exchanger that has the following requirements:

Hot fluid inlet temperature = 390 °F
Cold fluid inlet temperature = 100 °F
Hot fluid outlet temperature = 200 °F
Hot fluid Cp = 0.605 BTU/lb °F
Hot fluid flow rate = 43800 lb/hr
Cold fluid Cp = 0.490 BTU/lb °F
Cold fluid flow rate = 149000 lb/hr
Inside heat transfer coefficient = 169 BTU/ft^2-hr-°F
Outside heat transfer coefficient = 109 BTU/ft^2-hr-°F
Dirt factor (Rd) = 0.00348 ft^2-hr-°F/BTU
Tube length = 16 ft
Tube diameter = 0.0625 ft

The Mdt,th option calculates Q (5,034,810 BTU/hr) and stores it for use by the GEO option.

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨EXC⟩	HEAT EXCHANGER
Select English units	⟨ENG⟩	HEAT EXCHANGER
Select log mean temperature difference	⟨MdT⟩	LOG MN TEMP DIFF
Enter incoming temperatures	390 ⟨thi⟩ 100 ⟨tci⟩ ⟨EOD⟩	KNOWN EXIT QTYS

(continued)

Example (Continued)

Procedure	Press		Display
Indicate that the hot outgoing temperature is known	⟨th⟩		3.
Enter hot outgoing temperature	200 ⟨tho⟩ ⟨EOD⟩	tho =	200.
Enter the flow data and display the missing temperature	.605 ⟨Cph⟩ 43800 ⟨wh⟩ .49 ⟨Cpc⟩ 149000 ⟨wc⟩ ⟨EOD⟩	tco =	168.96
View the results	⟨-->⟩ ⟨MdT⟩ ⟨R⟩ ⟨S⟩ ⟨-->⟩ ⟨Ft1⟩ ⟨Ft2⟩	MdT = R = S = Ft1 = Ft2 =	152.6 2.755 0.238 0.894 0.976
Select geometry	⟨ESC⟩ ⟨ESC⟩ ⟨GEO⟩	GEOMETRY	
Enter the heat transfer coefficients	169 ⟨hio⟩ 109 ⟨ho⟩ ⟨EOD⟩	ho =	109.
Enter the dirt factor	.00348 ⟨Rd⟩	Rd =	0.00348
Accept the entries for Q, Ft, and MdT	⟨EOD⟩		0.
View the design factors of the heat exchanger	⟨Uo⟩ ⟨Ud⟩ ⟨A⟩	Uo = Ud = A =	66.2626 53.846 685.3894
Calculate the number of tubes	⟨-->⟩ 16 ⟨LEN⟩ .0625 ⟨DIA⟩ ⟨EOD⟩	# TUBES =	218.17

Example 3: Calculating Pressure Drop

The following example illustrates how to use the Heat Exchanger Design program to calculate pressure drop.

Example

Determine the tube-side and shell-side pressure drop for an exchanger with the following specifications:

Parameter	Tube-Side	Shell-Side
Flow rate, lb/hr	280000	175000
Fluid Viscosity, lb/ft-hr	2.23	1.96
No. of Tubes	160	—
No. of Passes	2	1
Tube ID, inches	0.68	—
Tube Length, inches	192	192
Tube Roughness, ft	0.00015	—
Fluid Specific Gravity	1	1
Shell ID, inches	—	15.25
Tube OD, inches	0.75	—
Baffle Spacing, inches	—	12
Tube Pitch, inches	0.9375	—
Fluid Density, lb/ft^3	62.4	62.4
Tube Arrangement	triangular	—

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨EXC⟩	HEAT EXCHANGER
Select English units	⟨ENG⟩	HEAT EXCHANGER
Select pressure drop	⟨dP⟩	PRESSURE DROP
Enter the conditions	280000 ⟨w⟩ 2.23 ⟨MU⟩ ⟨EOD⟩	SELECT SIDE
Select tube side	⟨TUB⟩	TUBE SIDE
Enter the tube data	160 ⟨#T⟩ 2 ⟨#P⟩ .68 ⟨ID⟩ ⟨EOD⟩	ID= 0.68

(continued)

Example (Continued)

Procedure	Press	Display
Enter the remaining tube data and display the tube-side pressure drop	192 ⟨LEN⟩ .00015 ⟨e⟩ 1 ⟨spg⟩ ⟨EOD⟩	dP = 6.25
Repeat program for shell-side pressure drop	⟨ESC⟩	PRESSURE DROP
Enter the shell-side flow rate and viscosity	175000 ⟨w⟩ 1.96 ⟨MU⟩ ⟨EOD⟩	SELECT SIDE
Select shell side	⟨SHL⟩	SHELL SIDE
Enter the shell-side data	1 ⟨#P⟩ 15.25 ⟨ID⟩ .75 ⟨OD⟩ 12 ⟨BSP⟩ ⟨EOD⟩	BSP = 12.
Enter the remaining data	192 ⟨LEN⟩ .9375 ⟨PIT⟩ 62.4 ⟨RHO⟩ ⟨EOD⟩	SELECT PITCH
Select triangular pitch and display the shell-side pressure drop	⟨TRI⟩	dP = 7.61

Chapter 11: Heat Transfer Coefficient Estimation

This chapter describes how to use the Heat Transfer Coefficient Estimation program, which estimates heat transfer coefficients for various configurations of heat transfer.

Table of Contents

Heat Transfer Coefficient Introduction

The program estimates heat transfer coefficients for four different geometries: 1) internal fluid-to-wall coefficients in turbulent flow, 2) external fluid-to-wall coefficients in a heat exchanger bundle, 3) external condensing coefficients on vertical tubes, and 4) external condensing coefficients on horizontal tubes.

Units Used in the Program

This program uses a number of standard correlations. Wherever possible, the correlations are dimensionless so that you may use either cgs (cal/cm^2-sec-°C) or engineering (BTU/ft^2-hr-°F) units for input variables. However, some of the correlations are intrinsically dimensional. Engineering units are used for the dimensional correlations, and the estimated coefficients are also in these units.

Internal Fluid-to-Wall Heat Transfer Coefficient

The Sieder-Tate[1] equation is used to estimate the internal fluid-to-wall heat transfer coefficient in turbulent flow. The equation is in dimensionless form so you may use any consistent set of units.

$$h_i = \frac{k}{D_i}(Re)^{0.8}(Pr)^{1/3}(0.023)$$

where

$$Re = \frac{\dot{m}}{\mu D_i}$$

External Fluid-to-Wall Heat Transfer Coefficient

This program uses the Donohue[2] method for estimating the external fluid-to-wall heat transfer coefficient in a heat exchanger bundle. This method requires that you specify both fluid properties and exchanger geometry. The equation is in dimensionless form, which allows you to use any consistent set of units.

$$h_i = 0.2\frac{k}{D_o}Re^{0.6}Pr^{1/3}$$

where

$$Re = \frac{D_o G_e}{\mu} \qquad G_e = (G_b G_s)^{1/2}$$

$$G_b = \frac{\dot{m}}{S_b} \qquad S_b = 0.1955\frac{\pi D_s^{\,2}}{4} - (.1955N_t)\frac{\pi D_o^{\,2}}{4}$$

$$G_s = \frac{\dot{m}}{S_c} \qquad S_c = PD_s\left(1 - \frac{D_o}{P_t}\right)$$

Laminar Film Condensation on Vertical Tubes

This program uses the Nusselt[3] equation for vertical tubes to calculate the external condensing coefficient. The correlation requires fluid properties, wall or tube length, and an estimate of the fluid-to-wall temperature difference.

$$h = 0.943\left(\frac{g_c k \rho \Delta H_v}{L \mu \Delta T}\right)^{1/4}$$

This correlation is inherently dimensional. Use engineering units throughout and convert to cgs units after calculating the heat transfer coefficient.

Laminar Film Condensation on Horizontal Tubes

This program uses the Nusselt[3] equation for film condensation on horizontal tubes to estimate the external fluid-to-wall heat transfer coefficient. The equation requires values for fluid properties, tube geometry, and the fluid-to-wall temperature difference.

$$h = 0.725\left(\frac{g_c k \rho \Delta H_v}{D_o \mu \Delta T}\right)^{1/4}$$

This equation is inherently dimensional; convert from engineering to cgs units, if necessary.

References

[1] Sieder, E. N., and Tate, G. E. 1936. Heat Transfer and Pressure Drop of Liquids in Tubes. *Industrial and Engineering Chemistry* 28: 1429.

[2] Donohue, D. A. 1949. Heat Transfer and Pressure Drop in Heat Exchangers. *Ind. Eng. Chem.* 11: 2499.

[3] Nusselt, W. 1916. Heat Conduction in Tubes. *VDI Z* 60: 541.

The following procedure provides instructions for using the Heat Transfer Coefficient Estimation program.

Before You Select the Program

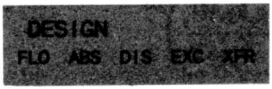
Before you select this program, you need values for specific heat, viscosity, density, and possibly latent heat of vaporization.

- If you do not have the values for specific heat, viscosity, and density, obtain them from the specific heat, viscosity and density programs (pages 6–21, 4–2, and 4–26) before running this program.
- If you are analyzing heat transfer for a horizontal or vertical tube and you do not have the value for latent heat of vaporization, obtain it from the latent heat of vaporization program (page 5–19) before running this program.

Selecting the Program

To select the Heat Transfer Coefficient Estimation program:

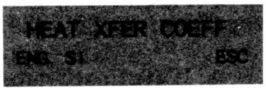
1. Select ⟨DSN⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨XFR⟩.

Selecting the Units

After you select the program, the following display appears.

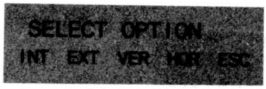


- If your entries and results are to be in the English system of units, press ⟨ENG⟩.
- If your entries and results are to be in the metric (SI, System International) system of units, press ⟨SI⟩.

If you run the program with one set of units and then return to this display and select the other set of units, the numbers you entered previously are converted automatically.

Selecting the Configuration

After you select the units, the program displays:



- If heat is being transferred to the wall of a tube from the fluid inside the tube (internal fluid), press ⟨INT⟩. The fluid must be in turbulent flow. The instructions for this option begin on the next page.

- If heat is being transferred to the wall of a crossflow tube from the fluid outside the tube (external fluid), press ⟨EXT⟩. The tube is usually part of a bundle inside a heat exchanger shell. Go to page 11–8 for the instructions for this option.

- If condensation is occurring on a vertical tube, press ⟨VER⟩. Go to page 11–11 for the instructions for this option.

- If condensation is occurring on a horizontal tube, press ⟨HOR⟩. Go to page 11–13 for the instructions for this option.

Entering the Internal Fluid-to-Wall Data

If you select the internal fluid-to-wall configuration, the program displays:

You can check the current entries by pressing INV ⟨w⟩, INV ⟨MU⟩, or INV ⟨Cp⟩. To enter the internal fluid-to-wall data:

1. Enter a value for the flow rate in either pounds per hour (English) or kilograms per hour (metric). Then press ⟨w⟩.

2. Enter a value for the viscosity of the fluid in either lb/ft-hr (English) or centipoise (metric). Then press ⟨MU⟩.

3. Enter a value for the specific heat in either BTU per pound °F (English) or calories per gram °C (metric). Then press ⟨Cp⟩.

4. If you enter an incorrect value, enter the correct value and press the corresponding key.

5. Press ⟨EOD⟩ to proceed with the program.

Entering the Internal Fluid-to-Wall Data (Continued)

where the message displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing [INV] ⟨k⟩ or [INV] ⟨IDp⟩.

6. Enter a value for the thermal conductivity of the fluid in either BTU per hour-ft-°F (English) or Watt per meter-°C (metric). Then press ⟨k⟩.

7. Enter a value for the inside diameter of the pipe in either ft (English) or meters (metric). Then press ⟨IDp⟩.

8. If you enter an incorrect value, enter the correct value and press the corresponding key.

9. Press ⟨EOD⟩ to proceed with the program.

Viewing the Result

After you enter the internal fluid-to-wall data, the program displays:

where xxxx is the value of the heat transfer coefficient expressed in BTU per hour-ft^2-°F (English) or in Watts per meter^2-°C (metric).

Entering the External Fluid-to-Wall Data

If you select the external fluid-to-wall crossflow configuration, the program displays:

You can check the current entries by pressing [INV] ⟨w⟩, [INV] ⟨MU⟩, or [INV] ⟨Cp⟩. To enter the internal fluid-to-wall data:

1. Enter a value for the flow rate in either pounds per hour (English) or kilograms per hour (metric). Then press ⟨w⟩.

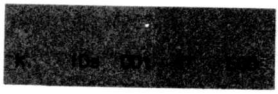
2. Enter a value for the viscosity of the fluid in either lb/ft-hr (English) or centipoise (metric). Then press ⟨MU⟩.

3. Enter a value for the specific heat in either BTU per pound °F (English) or calories per gram °C (metric). Then press ⟨Cp⟩.

4. If you enter an incorrect value, enter the correct value and press the corresponding key.

5. Press ⟨EOD⟩ to proceed with the program.

Entering the External Fluid-to-Wall Data (Continued)



where the message displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨k⟩, INV ⟨IDs⟩, INV ⟨ODt⟩, or INV ⟨#T⟩. To continue entering the internal fluid-to-wall data:

6. Enter a value for the thermal conductivity of the fluid in either BTU per hour-ft-°F (English) or Watt per meter-°C (metric). Then press ⟨k⟩.

7. Enter a value for the inside diameter of the shell in either ft (English) or meters (metric). Then press ⟨IDs⟩.

8. Enter a value for the outside diameter of the tube in either ft (English) or meters (metric). Then press ⟨ODt⟩.

9. Enter the number of tubes and press ⟨#T⟩.

10. If you enter an incorrect value, enter the correct value and press the corresponding key.

11. Press ⟨EOD⟩ to proceed with the program.

(continued)

Entering the External Fluid-to-Wall Data (Continued)

You can check the current entries by pressing INV ⟨TUB⟩ or INV ⟨BAF⟩. To continue entering the internal fluid-to-wall data:

12. Enter a value for the tube pitch in either tubes per ft (English) or tubes per meter (metric). Then press ⟨TUB⟩.

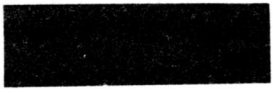
13. Enter a value for the baffle pitch in either baffles per ft (English) or baffles per meter (metric). Then press ⟨BAF⟩.

14. If you enter an incorrect value, enter the correct value and press the corresponding key.

15. Press ⟨EOD⟩ to proceed with the program.

Viewing the Result

After you enter the external fluid-to-wall data, the program displays:



where xxxx is the value of the heat transfer coefficient expressed in BTU per hour-ft^2-°F (English) or in Watts per $meter^2$-°C (metric).

Entering the Vertical Tube Data

If you select the condensing on a vertical tube configuration, the program displays:

You can check the current entries by pressing [INV] ⟨k⟩, [INV] ⟨MU⟩, or [INV] ⟨RHO⟩. To enter the vertical tube data:

1. Enter a value for the thermal conductivity of the condensed liquid in either BTU per hour-ft-°F (English) or Watt per meter-°C (metric). Then press ⟨k⟩.

2. Enter a value for the viscosity of the condensed liquid in either lb/ft-hr (English) or centipoise (metric). Then press ⟨MU⟩.

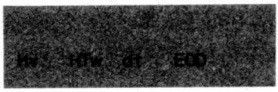
3. Enter a value for the density of the condensed liquid in either lb/ft^3 (English) or g/cm^3 (metric). Then press ⟨RHO⟩.

4. If you enter an incorrect value, enter the correct value and press the corresponding key.

5. Press ⟨EOD⟩ to proceed with the program.

(continued)

Entering the Vertical Tube Data (Continued)



where the value displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨Hv⟩, INV ⟨HTw⟩, or INV ⟨dt⟩.

6. Enter a value for the heat of vaporization in either BTU per pound (English) or kilojoules per kilogram (metric). Then press ⟨Hv⟩.

7. Enter a value for the wall height in either feet (English) or meters (metric). Then press ⟨HTw⟩.

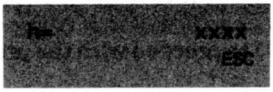
8. Enter a value for the change in temperature in either °F (English) or °C (metric). Then press ⟨dt⟩.

9. If you enter an incorrect value, enter the correct value and press the corresponding key.

10. Press ⟨EOD⟩ to proceed with the program.

Viewing the Result

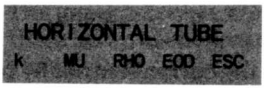
After you enter the vertical tube data, the program displays:



where xxxx is the value of the heat transfer coefficient expressed in BTU per hour-ft^2-°F (English) or in Watts per meter^2-°C (metric).

Entering the Horizontal Tube Data

If you select the condensing on a horizontal tube configuration, the program displays:



You can check the current entries by pressing INV ⟨k⟩, INV ⟨MU⟩, or INV ⟨RHO⟩. To enter the horizontal tube data:

1. Enter a value for the thermal conductivity of the condensed liquid in either BTU per hour-ft-°F (English) or Watt per meter-°C (metric). Then press ⟨k⟩.

2. Enter a value for the viscosity of the condensed liquid in either lb/ft-hr (English) or centipoise (metric). Then press ⟨MU⟩.

3. Enter a value for the density of the condensed liquid in either lb/ft^3 (English) or g/cm^3 (metric). Then press ⟨RHO⟩.

4. If you enter an incorrect value, enter the correct value and press the corresponding key.

5. Press ⟨EOD⟩ to proceed with the program.

(continued)

Entering the Horizontal Tube Data (Continued)

where the value displayed when this menu first appears is left over from the previous menu.

You can check the current entries by pressing INV ⟨Hv⟩, INV ⟨ODt⟩, or INV ⟨dt⟩. To continue entering the horizontal tube data:

6. Enter a value for the heat of vaporization in either BTU per pound (English) or kilojoules per kilogram (metric). Then press ⟨Hv⟩.

7. Enter a value for the outside diameter of the tube in either feet (English) or meters (metric). Then press ⟨ODt⟩.

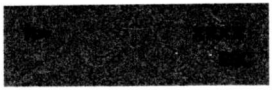
8. Enter a value for the temperature difference between the wall and the bulk vapor in either °F (English) or °C (metric). Then press ⟨dt⟩.

9. If you enter an incorrect value, enter the correct value and press the corresponding key.

10. Press ⟨EOD⟩ to proceed with the program.

Viewing the Result

After you enter the horizontal tube data, the program displays:



where xxxx is the value of the heat transfer coefficient expressed in BTU per hour-ft^2-°F (English) or in Watts per $meter^2$-°C (metric).

Example 1: Internal Fluid-to-Wall Heat Transfer

The following example illustrates how to use the internal fluid-to-wall option of the Heat Transfer Coefficient Estimation program.

Example

Estimate the internal fluid-to-wall heat transfer coefficient for fluid n-hexane flowing at a rate of 1000 pounds per hour through a two-inch, Schedule-40 pipe. The average temperature of the n-hexane is 100 °F, and there is sufficient pressure in the line to prevent any vaporization.

Physical Property Data:

Viscosity = 0.806 lb/ft-hr
Heat Capacity = 0.556 BTU/lb-°F
Thermal Conductivity = 0.0772 BTU/hr-ft-°F
Inside Pipe Diameter = 0.1723 ft

Procedure	Press	Display
Select program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨XFR⟩	HEAT XFER COEFF
Select English units	⟨ENG⟩	SELECT OPTION
Select the internal fluid-to-wall option	⟨INT⟩	INT FLUID->WALL
Enter the internal fluid-to-wall data	1000 ⟨w⟩ .806 ⟨MU⟩ .556 ⟨Cp⟩ ⟨EOD⟩ .0772 ⟨k⟩ .1723 ⟨IDp⟩ ⟨EOD⟩	h= 22.57

Example 2: Heat Transfer of Crossflow Tubes

The following example illustrates how to use the external fluid-to-wall option of the Heat Transfer Coefficient Estimation program.

Example

Liquid hexane is heated on the shell side of a tubular exchanger at an average rate of 80,000 lb/hr at an average temperature of 100 °F.

Physical Property Data:

Viscosity = 0.806 lb/ft-hr
Heat Capacity = 0.556 BTU/lb- °F
Thermal Conductivity = 0.0772 BTU/hr-ft- °F

The heat exchanger has the following specifications:

Shell Inside Diameter = 2.9167 ft
Tube Outside Diameter = 0.0625 ft
Number of Tubes = 828

The tubes are on a 1-inch square pitch. Standard 25 percent baffles are spaced 12 inches apart. Estimate the individual external heat transfer coefficient for the hexane.

Procedure	Press	Display
Select the program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨XFR⟩	HEAT XFER COEFF
Select English units	⟨ENG⟩	SELECT OPTION
Select the external fluid-to-wall option	⟨EXT⟩	EXT FLUID->WALL
Enter the internal fluid-to-wall data	80000 ⟨w⟩ .806 ⟨MU⟩ .556 ⟨Cp⟩ ⟨EOD⟩ .0772 ⟨k⟩ 2.9167 ⟨IDs⟩ .0625 ⟨ODt⟩ 828 ⟨#T⟩ ⟨EOD⟩	ENTER PITCH
Enter the tube and baffle pitches	1 ⟨TUB⟩ 12 ⟨BAF⟩ ⟨EOD⟩	h= 31.31

Example 3: Condensing on a Vertical Tube

The following example illustrates how to use the vertical tube option of the Heat Transfer Coefficient Estimation program.

Example

Estimate the heat transfer coefficient for condensing n-hexane at an average temperature of 100 °F.

Physical Property Data:

Thermal Conductivity = 0.0772 BTU/hr-ft-°F
Viscosity = 0.806 lb/ft-hr
Density = 40.25 lb/ft^3
Latent Heat of Vaporization = 155 BTU/lb

The fluid-to-wall temperature difference is 50 °F and the wall is 2 feet high.

Procedure	Press	Display
Select the program	RUN ⟨CHE⟩ ⟨DSN⟩ ⟨XFR⟩	HEAT XFER COEFF
Select English units	⟨ENG⟩	SELECT OPTION
Select the vertical tube option	⟨VER⟩	VERTICAL TUBE
Enter the vertical tube data	.0772 ⟨k⟩ .806 ⟨MU⟩ 40.25 ⟨RHO⟩ ⟨EOD⟩ 155 ⟨Hv⟩ 2 ⟨HTw⟩ 50 ⟨dt⟩ ⟨EOD⟩	h = 147.45

Example 4: Condensing on a Horizontal Tube

The following example illustrates how to use the horizontal tube option of the Heat Transfer Coefficient Estimation program.

Example

Estimate the heat transfer coefficient for condensing n-hexane at 100 °F and a fluid-to-wall temperature difference of 25 °F. The tube is one-inch, Schedule-40 pipe.

Physical Property Data:

Thermal Conductivity = 0.0772 BTU/ft-hr-°F
Viscosity = 0.806 lb/ft-hr
Density = 40.25 lb/ft^3
Latent Heat of Vaporization = 155 BTU/lb
Tube Outside Diameter = 0.1096 ft

Procedure	Press	Display
Select program	RUN ⟨CHE⟩	
	⟨DSN⟩ ⟨XFR⟩	HEAT XFER COEFF
Select English units	⟨ENG⟩	SELECT OPTION
Select the vertical tube option	⟨HOR⟩	HORIZONTAL TUBE
Enter the horizontal tube data	.0772 ⟨k⟩ .806 ⟨MU⟩	
	40.25 ⟨RHO⟩ ⟨EOD⟩	
	155 ⟨Hv⟩ .1096 ⟨ODt⟩	
	25 ⟨dt⟩ ⟨EOD⟩	h= 278.63

Chapter 12: Other Chemical Engineering Solutions

This chapter describes how to use the Equilibrium Flash Calculation program and the Activity Coefficient program.

Table of Contents

Equilibrium Flash Introduction

The Equilibrium Flash program takes a feed stream at a given composition, temperature, and pressure and performs a single-stage, equilibrium flash calculation. The program requires you to enter the equilibrium K-values for the system at the temperature and pressure of the flash.

Method of Calculation

The equilibrium flash calculation consists of an iterative solution to the expression

$$\sum_{i=1}^{n} \frac{z_i(K_i - 1)}{V(K_i - 1) + F} = 0$$

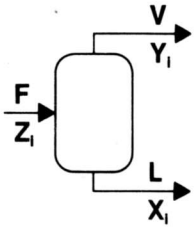
where n is the number of components.

The flash equation is derived from the following fundamental relations.

Total mass balance:
$F = V + L$

Component balance:
$z_i F = x_i L + y_i V$

Equilibrium relation:
$y_i = K_i * x_i$



The program uses the iterative method suggested by Mansouri to solve the flash equation. When you provide K-values corresponding to a given temperature, the program calculates the liquid (L) and vapor (V) molar split and the composition of each phase.

Bubble Point and Dew Point

To calculate the bubble point of the mixture, you must determine the temperature where L = 0.9995. To calculate the dew point, you must determine the temperature where V = 0.9995.

Reference

Mansouri, S. 1979. Streamline Flash Computations with Calculator Program. *Chemical Engineering* 18: 99.

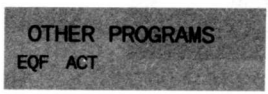
The Equilibrium Flash Calculation Program

The following procedure provides instructions for using the Equilibrium Flash Calculation program.

Selecting the Program

To select the Equilibrium Flash Calculation program:

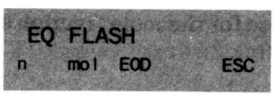
1. Select ⟨OTH⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨EQF⟩.

Defining the Mixture

After you select the program, the following display appears.

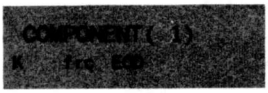


You can check the current entries by pressing INV ⟨n⟩ or INV ⟨mol⟩. To define the mixture:

1. Enter the number of components in the mixture and press ⟨n⟩.
2. Enter a value for the feed rate in moles per time and press ⟨mol⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.

Entering the Properties

After you define the mixture, the program prompts you to enter the volatility and mole fraction for the first component.



You can check the current entries by pressing INV ⟨K⟩ or INV ⟨frc⟩. To define the mixture:

1. Enter a value for the relative volatility of the component and press ⟨K⟩.
2. Enter a value for the mole fraction of the component and press ⟨frc⟩.
3. If you enter an incorrect value, enter the correct value and press the corresponding key.
4. Press ⟨EOD⟩ to proceed with the program.
5. Repeat steps 1 through 4 for each component except the last.

For the last component, you enter only the relative volatility. Because the total of all the mole fractions of a mixture must be one, the program determines the last mole fraction without your entering it.

Obtaining the Results

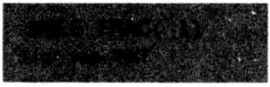
After the program determines the last mole fraction, the program displays:

⟨liq⟩ Displays the production rate of liquid in moles per time. The units of liq are the same as the units of mol.

⟨vap⟩ Displays the production rate of vapor in moles per time. The units of vap are the same as the units of mol.

To display the results:

1. Press the key that corresponds to the production rate you want to view.
2. Press ⟨-->⟩ to proceed with the program.



⟨liq⟩ Displays the mole fraction of the component in the liquid.

⟨vap⟩ Displays the mole fraction of the component in the vapor.

3. Press the keys that correspond to the results you want to view for this component.
4. Press ⟨NXT⟩ to advance to the next component.
5. Repeat steps 3 and 4 for each component.

Example: Calculating Equilibrium Flash

The following example illustrates how to use the Equilibrium Flash Calculation program.

Example

Find the compositions and production rates of the liquid and vapor phases caused by flashing the mixture given below. The feed rate is 100 moles per hour and the flash conditions are 54.6 °C and 11.22 atm.

Component	K-Value	Mole Fraction
Ethane	4.2	0.087
Methane	1.6	0.202
i-Butane	0.74	0.696
n-Butane	0.21	0.015

Procedure	Press	Display
Select the program	RUN ⟨CHE⟩ ⟨OTH⟩ ⟨EQF⟩	EQ FLASH
Define the mixture	4 ⟨n⟩ 100 ⟨mol⟩ ⟨EOD⟩	COMPONENT(1)
Enter the K-value and mole fraction for each component	4.2 ⟨K⟩ .087 ⟨frc⟩ ⟨EOD⟩	COMPONENT(2)
	1.6 ⟨K⟩ .202 ⟨frc⟩ ⟨EOD⟩	COMPONENT(3)
	.74 ⟨K⟩ .696 ⟨frc⟩ ⟨EOD⟩	COMPONENT(4)
	.21 ⟨K⟩ ⟨EOD⟩	FRACTION FEED:
View the production rates	⟨liq⟩	liq = 59.8145
	⟨vap⟩	vap = 40.1855
View the component fractions	⟨--->⟩ ⟨liq⟩	liq = 0.0381
	⟨vap⟩	vap = 0.1598
	⟨NXT⟩ ⟨liq⟩	liq = 0.1628
	⟨vap⟩	vap = 0.2604
	⟨NXT⟩ ⟨liq⟩	liq = 0.7772
	⟨vap⟩	vap = 0.5751
	⟨NXT⟩ ⟨liq⟩	liq = 0.0220
	⟨vap⟩	vap = 0.0046

Activity Coefficient Introduction

The Activity Coefficient program estimates liquid-phase activity coefficients for mixtures using the Wilson equation.

Method of Estimation

The program calculates liquid-phase activity coefficients for multicomponent mixtures. This program uses the Wilson equation[1]:

$$\ln\gamma_i = -\ln\left(\sum_j x_j\Lambda_{ij}\right) + 1 - \sum_k \frac{x_k\Lambda_{ki}}{\sum_j x_j\Lambda_{kj}}$$

You must provide the binary interaction coefficients (Λ) for binary pairs in the mixture. Reference 2 is an excellent resource for these coefficients.

Reference

[1] Wilson, G.M. 1964. Vapor-Liquid Equilibrium, XI, A New Expression for the Excess Free Energy of Mixing. *Journal of the American Chemical Society* 2: 127.

[2] Hirata, M.; Ohe, S.; and Nagahama, K. 1975. *Computer Aided Data Book of Vapor-Liquid Equilibria*. New York: Elsevier Scientific Publishing Co.

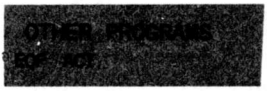
The Activity Coefficient Program

The following procedure provides instructions for using the Activity Coefficient program.

Selecting the Program

To select the Activity Coefficient program:

1. Select ⟨OTH⟩ from the **CHEM ENGINEERING** menu. The program displays:



2. Select ⟨ACT⟩.

Defining the Mixture

After you select the program, the following display appears.

You can check the current entry by pressing **INV** ⟨n⟩. To define the mixture:

1. Enter the number of components in the mixture and press ⟨n⟩.
2. If you enter an incorrect value, enter the correct value and press ⟨n⟩.
3. Press ⟨EOD⟩ to proceed with the program.

Entering the Mole Fractions

After you define the mixture, the program displays:

You can check the current entry by pressing [CE]. To enter the mole fractions:

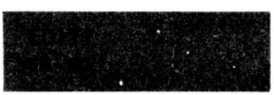
1. Enter the mole fraction of the indicated component and press ⟨ENT⟩.

2. Repeat step 1 for each component except the last.

Because the total of all the mole fractions of a mixture must be one, the program determines the last mole fraction without your entering it.

Editing the Mole Fractions

After the program determines the last mole fraction, it displays:



- If you want to edit a value, press ⟨YES⟩ and return to the top of this page.

- If you do not want to edit any values, press ⟨NO⟩ and go to the next page.

Entering the Interactions

After you select not to edit, the program displays:

```
L( 1, 2)
ENT
```

To enter the interactions:

1. Enter the binary interaction coefficient for the component pair indicated and press ⟨ENT⟩.
2. Repeat step 1 for each binary interaction coefficient as prompted.

Editing the Interactions

After you enter the last interaction, the program displays:

```
EDIT
i~j  ENT  EOD
```

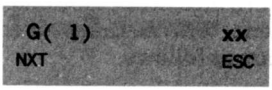
To edit an interaction:

1. Enter a value for i and press [x~t].
2. Enter a value for j and press ⟨i~j⟩. The value for Λ_{ij} is displayed.
3. If the value for Λ_{ij} is correct, press ⟨ENT⟩. Otherwise, enter the correct value and press ⟨ENT⟩.
4. Repeat steps 1, 2, and 3 for each binary interaction you want to edit.

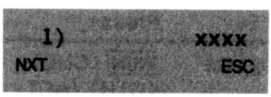
When you finish editing the interactions, press ⟨EOD⟩.

Obtaining the Results

After you finish editing, the program displays:



which scrolls to



where xxxx is the indicated liquid activity coefficient.

To obtain the results:

1. View this liquid activity coefficient.
2. Press ⟨NXT⟩ to advance to the next coefficient.
3. Repeat steps 1 and 2 for each coefficient.

If you advance past the last coefficient, the program returns to the first coefficient.

Example: Calculating Activity Coefficients

The following example illustrates how to use the Activity Coefficient program.

Example

Find the liquid-phase activity coefficients for methanol and benzene in a mixture of .4061 moles methanol and the rest benzene. With methanol as component 1, the interactions are as follows.

$\Lambda_{1,2} = 0.18702$ $\Lambda_{2,1} = 0.52058$

Procedure	Press	Display
Select the program	RUN ⟨CHE⟩ ⟨OTH⟩ ⟨ACT⟩	ACTIVITY COEFF
Define the mixture	2 ⟨n⟩ ⟨EOD⟩	x(1)
Enter the mole fraction for each component except the last	.4061 ⟨ENT⟩ ⟨NO⟩	L(1, 2)
Enter the 1,2 interaction	.18702 ⟨ENT⟩	L(2, 1)
Enter the 2,1 interaction	.52058 ⟨ENT⟩	EDIT
View the first result (the display scrolls)	⟨EOD⟩	G(1) = 1.6326910 1) = 1.632691076
View the next result (the display scrolls)	⟨NXT⟩	G(2) = 1.3940239 2) = 1.394023943

Appendix A: Reference Information

The register contents provided in this chapter are important when you need to save and retrieve data. The list of flags used in each program is important during programming and debugging. The table of compounds gives you an alternative to the alphabetical list of compounds in Chapter 1.

Table of Contents

The following table lists the contents of each data register. Using these tables, you can determine which data register is occupied by any value a program generates. You can also determine the block of registers to save for those programs that can use stored data.

Physical Properties

Program Name	Register	Contents
Properties Table	A	used
	B	Tc
	C	Pc
	D	Vc
	E	Tb
	F	w
	G	CpA
	H	CpB
	I	CpC
	J	Cpn
	K	CpD
	L	Zra
	M	Mw
	N	# of compound
Gas Viscosity of a Pure Gas	A	used
	B	tc
	C	Pc
	D	Vc
	E	t
	F	used
	G	RHO
	H	used
	I	used
	J	MU (low)
	K	MU (high)
	L	used
	M	Mw
	N	# of compound
	O	Tr
	P	(G*D) = P

Physical Properties (Continued)

Program Name	Register	Contents
Gas Viscosity of a Gas Mixture	A	used
	B	used
	C	used
	D	used
	E	t
	F	used
	G	used
	H	used
	I	used
	J	used
	K	used
	L	n
	M	used
	N	used
	O	used
	P (015)	used
	016	frc(1)
	017	Tc(1)
	018	Vc(1)
	019	Zc(1)
	020	Mw(1)
	:	:
	15 + 5n	Mw(n)

(continued)

	Program Name	Register	Contents
Physical Properties (Continued)	Gas Thermal Conductivity	A	used
		B	used
		C	used
		D	n
		E	used
		F	P
		G	used
		H	t
		I	used
		J	used
		K	used
		L	lambda
		M	used
		N	used
		O	used
		P	used
		Q	used
		R	used
		S	used
		T	used
		U	used
		V(021)	used
		022	x(1)
		023	Tc(1)
		024	Pc(1)
		025	Mw(1)
		026	Cp(1)
		027	Z(1)
		028	Zc(1)
		029	Tb(1)
		030	MU(1)
		031	used
		:	:
		21 + 10n	used

Physical Properties (Continued)

Program Name	Register	Contents
Liquid Viscosity	A	used
	B	tc
	C	Pc
	D	used
	E	t
	F	w
	G	RHO(1) or RHO
	H	RHO(2)
	I	MU(1)
	J	MU(2)
	K	GCa
	L	GCb
	M	Mw
	N	# of compound
	O	Tr = E/B
	P	theta
	Q	n
	R	x1
	S	1 – x1
	T	used
	U	used
	V	used
	W	used
	X	used
	Y	used
	Z	used

(continued)

	Program Name	Register	Contents
Physical Properties (Continued)	Liquid Thermal Conductivity	A	used
		B	used
		C	used
		D	n
		E	used
		F	used
		G	used
		H	t
		I	used
		J	used
		K	used
		L	lambda
		M	used
		N (013)	used
		014	x(1)
		015	Tc(1)
		016	Tb(1)
		017	H(1)
		018	Hvb(1)
		019	Cp(1)
		020	RHO(1)
		021	Mw(1)
		:	:
		13 + 8n	Mw(n)

Physical Properties (Continued)

Program Name	Register	Contents
Liquid Density	A	used
	B	used
	C	used
	D	n
	E	t
	F	used
	G	used
	H	used
	I	RHO
	J	used
	K	available
	L	used
	M	used
	N (013)	# of component
	014	x(1)
	015	Pc(1)
	016	Tc(1)
	017	Zra(1)
	018	Mw(1)
	:	:
	13 + 5n	Mw(n)
PvK	A	used
	B	Tc
	C	Pc
	D	T
	E	Tb
	F	Pv
	G	Kr
	H	used
	I	used
	J	used
	K	.005 = G
	L	used
	M	P
	N	# of compound

(continued)

	Program Name	Register	Contents
Physical Properties (Continued)	Critical Properties	A	used
		B	used
		C	available
		D	inc
		E	tb
		F	n
		G	tc
		H	Pc
		I	Vc
		J	used
		K	used
		L	used
		M	Mw
	Latent Heat of Vaporization	A	used
		B	Tc
		C	Pc
		D	T
		E	Tb
		F	ΔHvb
		G	ΔHvt
		H	used
		I	used
		J	used
		K	used
		L	used
		M	Mw
		N	# of compound

	Program Name	Register	Contents
Thermodynamics	SRK	A	used
		:	:
		D	used
		E	available
		F	w
		G	available
		:	:
		J	available
		K	pressure
		L	Tb
		M	Mw
		N	# of compound
		O	used
		P	available
		Q	used
		R	available
		S	(n) no. of components
		T	used
		U	used
		V	t
		W	available
		X	available
		Y	available
		Z(025)	Z
		026	Mw(1)
		:	:
		25+n	Mw(n)
		26+n	x(1)
		:	:
		25+2n	x(n)
		26+2n	Pc(1)
		:	:
		25+3n	Pc(n)
		26+3n	Tc(1)
		:	:
		25+4n	Tc(n)
		26+4n	w(1)
		:	:
		25+5n	w(n)
		26+5n	used
		:	:
		25+7n	used

(continued)

	Program Name	Register	Contents
Thermodynamics (Continued)	Peng-Robinson	A	used
		:	:
		D	used
		E	available
		F	w
		G	available
		:	:
		J	available
		K	pressure
		L	Tb
		M	Mw
		N	# of compound
		O	used
		P	available
		Q	used
		R	available
		S	(n) no. of components
		T	used
		U	used
		V	t
		W	available
		X	available
		Y	available
		Z(025)	Z
		026	Mw(1)
		:	:
		25+n	Mw(n)
		26+n	x(1)
		:	:
		25+2n	x(n)
		26+2n	Pc(1)
		:	:
		25+3n	Pc(n)
		26+3n	Tc(1)
		:	:
		25+4n	Tc(n)

	Program Name	Register	Contents
Thermodynamics (Continued)	Peng-Robinson (Continued)	26 + 4n	w(1)
		:	:
		25 + 5n	w(n)
		26 + 5n	used
		:	:
		26 + 9n + n(n − 1)/2	used
	Specific Heat	A	used
		B	tc
		C	Pc
		D	used
		E	t
		F	w
		G	A
		H	B
		I	C
		J	n
		K	D
		L	P
		M	Mw
		N	# of compound
		O	Tr
		P	Pr
		Q	uncorrected Cpg
		R	Cpl
		S	dCp0
		T	dCp1
		U	corrected Cpg

	Program Name	Register	Contents
Equipment Design	Pipe Design for Liquid Flow	A	.005
		B	K1
		C	K2
		D	conversion
		E	f
		F	used
		G	used
		H	used
		I	ΔP
		J	Q
		K	RHO
		L	MU
		M	D
		N	e
		O	L
		P	ΔZ
		Q	ΣLe/D
		R	Re
		S	V_{i+1}
		T	V_i
		U	Le/D(L)
		V	Le/D(U)
		W	Le/D(T->)
		X	Le/D(->T)
		Y	Le/D(GTE)
		Z	Le/D(GLB)

Program Name	Register	Contents
Absorber Design	A	used
	:	:
	H	used
	I	t1
	J	tN
	K	N
	L	M = #C
	M	t_0
	N	t_{N+1}
	O	L_{N+1}
	P	V_0
	Q	L1
	R	LN
	S	V1
	T(019)	VN
	020	Eff(1)
	:	:
	19+N	Eff(N)
	20+N	Entering xl(1)
	:	:
	19+N+M	Entering xl(M)
	20+N+M	Entering xg(1)
	:	:
	19+N+2M	Entering xg(M)
	20+N+2M	Recovery(1)
	:	:
	19+N+3M	Recovery(M)
	20+N+3M	Cpl(1)
	:	:
	19+N+4M	Cpl(M)
	20+N+4M	Cpv(1)
	:	:
	19+N+5M	Cpv(M)
	20+N+5M	ΔHv(1)
	:	:
	19+N+6M	ΔHv(M)
	20+N+6M	K(1)
	:	:
	19+N+7M	K(M)

(continued)

	Program Name	Register	Contents
Equipment Design (Continued)	Distallation Design	A	used
		B	available
		C	used
		D	available
		:	:
		J	available
		K	# of components
		L	light key
		M	feed condition
		N	Act.:min. multiplier
		O	Nmin
		P	Rmin
		Q	N
		R	Klk feed
		S	Khk feed
		T	Klk vapor
		U	Khk vapor
		V	Klk bottoms
		W	Khk bottoms
		X	Klk condenser
		Y	xlk bottoms
		Z (025)	xhk bottoms
		026	Khk condenser
		027	available
		028	available
		029	feed x(1)
		:	:
		28 + N	feed x(N)
		29 + N	distillate x(1)
		:	:
		28 + 2N	distillate x(N)
		29 + 2N	t_{avg} K(1)
		:	:
		28 + 3N	t_{avg} K(N)

	Program Name	Register	Contents
Equipment Design (Continued)	Heat Exchanger Design	A	option
		B	B1 in dP
		C	C in dP
		D	T1 in dP
		E	0.0005
		F	F
		G	G
		H	R2
		I	available
		J	used
		K	Ti in MdT
		L	To in MdT
		M	ti in MdT
		N	to of Mdt
		O	wh
		P	wc
		Q	used
		R	R in MdT
		S	S in MdT
		T	LMTD
		U	Cph in MdT
		V	Cpc in MdT
		W	used
		X	Ft2 in MdT
		Y	hio in GEO
		Z(025)	ho in GEO
		026	Rd
		027	Uo
		028	Ud
		029	area
		030	length
		031	diameter
		032	w in dP
		033	MU in dP
		034	RHO in dP
		035	Sp. Gravity in dP
		036	Baffle spacing in dP

(continued)

	Program Name	Register	Contents
Equipment Design (Continued)	Heat Exchanger Design (Continued)	037	OD in dP
		038	ID in dP
		039	pitch in dP
		040	# tubes in dP
		041	e in dP
		042	#P in dP
		043	length in dP
	Heat Transfer Coefficient	A	available
		B	Thermal conductivity
		C	MU
		D	Flow rate
		E	RHO
		F	Cp
		G	Heat of vaporization
		H	Fluid –> wall ΔT
		I	Tube OD
		J	Shell ID
		K	Wall height
		L	Tube pitch
		M	Baffle pitch
		N	# of tubes
		O	Pipe ID
		P	Reynolds number

Other Programs

Program Name	Register	Contents
Equilibrium	swap	used
Flash	A	xl
	B	xv
	C	feed moles
	D	n
	E	.0005*C
	F	Vmid
	G	Vleft
	H	Vright
	I	f(Vleft)
	J	f(Vright)
	K	f(Vmid)
	L	used
	M	used
	N	used
	O	used
	P	available
	Q(016)	available
	017	K(1)
	018	x(1)
	019	xl(1)
	020	xv(1)
	021	K(2)
	:	:
	16+4n	xv(n)

(continued)

	Program Name	Register	Contents
Other Programs (Continued)	Activity	A	used
	Coefficient	B	used
		C	used
		D	n
		E	G(i)
		F	x(j)
		G	A(i,j)
		H	available
		I	used
		J	used
		K	used
		L	available
		:	:
		P(015)	available
		016	x(1)
		:	:
		15+n	x(n)
		16+n	G(1)
		:	:
		15+2n	G(n)
		16+2n	A(1,1)
		:	:
		15+3n	A(1,n)
		16+3n	A(2,1)
		:	:
		$15+2n+n^2$	A(n,n)

Flags Used

Some of the programs in the Chemical Engineering library use one or more flags. If you write a program that uses a flag and then run a program in the library, the status of the flag may change if it is one of the flags in the list below.

List of Flags

Programs in the Chemical Engineering library that use flags are listed below.

Program Name	Flag 16	Flag 17	Flag 18
Gas Viscosity	x	x	x
Gas Thermal Conductivity	x		
Liquid Viscosity	x		
SRK Thermodynamics	x		
P-R Thermodynamics	x		
Specific Heat	x	x	x
Pipe Design for Liq. Flow	x		
Heat Exchanger Design	x		
Heat Transfer Coefficient	x		

This table presents the built-in properties table by chemical category. The compound numbers are assigned according to their groupings into these categories.

	Name of Compound	Selection Number
Paraffinic Hydrocarbons	methane	1
	ethane	2
	propane	3
	n-butane	4
	i-butane	5
	n-pentane	6
	i-pentane	7
	neopentane	8
	n-hexane	9
	2-methylpentane	10
	3-methylpentane	11
	2,2-dimethylbutane	12
	2,3-dimethylbutane	13
	n-heptane	14
	2,2,3-trimethylbutane	15
	3-methylhexane	16
	3-ethylpentane	17
	2,3-dimethylpentane	18
	2,4-dimethylpentane	19
	3,3-dimethylpentane	20
	n-octane	21
	2,2,3,3-tetramethylbutane	22
	2-methylheptane	23
	3-methylheptane	24
	4-methylheptane	25
	3-ethylhexane	26
	2,2-dimethylhexane	27
	2,3-dimethylhexane	28
	2,4-dimethylhexane	29
	2,5-dimethylhexane	30
	3,3-dimethylhexane	31
	3,4-dimethylhexane	32
	2-methyl-3-ethylpentane	33
	3-methyl-3-ethylpentane	34
	2,3,3-trimethylpentane	35
	2,3,4-trimethylpentane	36

	Name of Compound	Selection Number
Paraffinic Hydrocarbons (Continued)	*n*-nonane	37
	2,2,5-trimethylhexane	38
	n-decane	39
	n-undecane	40
	n-dodecane	41
	n-tridecane	42
	n-tetradecane	43
	n-pentadecane	44
	n-hexadecane	45
	n-heptadecane	46
	n-octadecane	47
	n-nonadecane	48
	n-eicosane	49
Monoolefinic Hydrocarbons	ethylene	50
	propylene	51
	1-butene	52
	cis 2-butene	53
	trans 2-butene	54
	isobutene	55
	1-pentene	56
	cis 2-pentene	57
	trans 2-pentene	58
	2-methyl 1-butene	59
	3-methyl 1-butene	60
	2-methyl 2-butene	61
	1-hexene	62
	cis 2-hexene	63
	trans 2-hexene	64
	cis 3-hexene	65
	trans 3-hexene	66
	2-methyl 2-pentene	67
	cis 3-methyl 2-pentene	68
	trans 3-methyl 2-pentene	69
	cis 4-methyl 2-pentene	70
	trans 4-methyl 2-pentene	71

(continued)

	Name of Compound	Selection Number
Monoolefinic Hydrocarbons (Continued)	2,3-dimethyl 1-butene	72
	3,3-dimethyl 1-butene	73
	2,3-dimethyl 2-butene	74
	1-heptene	75
	1-octene	76
	1-nonene	77
	1-decene	78
	1-undecene	79
	1-dodecene	80
	1-tridecene	81
	1-tetradecene	82
	1-pentadecene	83
	1-hexadecene	84
	1-octadecene	85
Diolefinic Hydrocarbons	propadiene	86
	1,2-butadiene	87
	1,3-butadiene	88
	1,2-pentadiene	89
	trans 1,3-pentadiene	90
	1,4-pentadiene	91
	3-methyl 1,2-butadiene	92
	isoprene	93
Alkyl Cycloalkanes	cyclopropane	94
	cyclobutane	95
	cyclopentane	96
	methylcyclopentane	97
	ethylcyclopentane	98
	1,1-dimethylcyclopentane	99
	cis 1,2-dimethylcyclopentane	100
	trans 1,2-dimethylcyclopentane	101
	n-propylcyclopentane	102
	n-hexylcyclopentane	103
	n-heptylcyclopentane	104

	Name of Compound	Selection Number
Alkyl Cycloalkanes (Continued)	*n*-octylcyclopentane	105
	n-nonylcyclopentane	106
	n-decylcyclopentane	107
	n-dodecylcyclopentane	108
	n-tridecylcyclopentane	109
	n-tetradecylcyclopentane	110
	n-pentadecylcyclopentane	111
	n-hexadecylcyclopentane	112
	cyclohexane	113
	methylcyclohexane	114
	ethylcyclohexane	115
	1,1-dimethylcyclohexane	116
	cis 1,2-dimethylcyclohexane	117
	trans 1,2-dimethylcyclohexane	118
	cis 1,3-dimethylcyclohexane	119
	trans 1,3-dimethylcyclohexane	120
	cis 1,4-dimethylcyclohexane	121
	trans 1,4-dimethylcyclohexane	122
	n-propylcyclohexane	123
	n-butylcyclohexane	124
Alkyl Cyclo-enes	cyclopentene	125
	cyclohexene	126
Acetylenes	acetylene	127
	methylacetylene	128
	ethylacetylene	129
	dimethylacetylene	130
	1-pentyne	131

	Name of Compound	Selection Number
Alkyl Benzenes and Styrene	benzene	132
	toluene	133
	ethylbenzene	134
	o-xylene	135
	m-xylene	136
	p-xylene	137
	n-propylbenzene	138
	cumene	139
	1-methyl-2-ethylbenzene	140
	1-methyl-3-ethylbenzene	141
	1-methyl-4-ethylbenzene	142
	n-butylbenzene	143
	styrene	144
	biphenyl (diphenyl)	145
Halogenated Hydrocarbons	methyl chloride	146
	methylene chloride	147
	chloroform	148
	carbon tetrachloride	149
	vinyl chloride	150
	trichloroethylene	151
	perchloroethylene	152
	chloroethane	153
	1,1-dichloroethane	154
	1,2-dichloroethane	155
	1,1,2-trichloroethane	156
	allyl chloride	157
	1,2-dichloropropane	158
	phosgene	159
	acetyl chloride	160
	methyl fluoride	161
	carbon tetrafluoride (R14)	162
	vinyl fluoride	163
	1,1-difluoroethylene	164
	methyl bromide	165
	ethyl bromide	166

	Name of Compound	Selection Number
Halogenated Hydrocarbons (Continued)	chlorobenzene	167
	fluorobenzene	168
	bromobenzene	169
	iodobenzene	170
	hexafluorobenzene	171
	trichlorofluoromethane (R11)	172
	dichlorodifluoromethane (R12)	173
	chlorotrifluoromethane (R13)	174
	dichloromonofluoromethane (R21)	175
	chlorodifluoromethane (R22)	176
	1,1,2-trichloro-1,2,2-trifluoroethane (R113)	177
	1,2-dichloro-1,1,2,2-tetrafluoroethane (R114)	178
	trifluorobromomethane	179
Alcohols	methanol	180
	ethanol	181
	n-propanol	182
	isopropanol	183
	n-butanol	184
	isobutanol	185
	sec-butanol	186
	tert-butanol	187
	1-pentanol	188
	1-hexanol	189
	1-heptanol	190
	2-propanol	191
	cyclohexanol	192
	1-decanol	193
Glycols	ethylene glycol	194
	diethylene glycol	195
	1,2-propylene glycol	196
	glycerine	197
Organic Oxides	ethylene oxide	198
	propylene oxide	199

	Name of Compound	Selection Number
Organic Acids	formic acid	200
	acetic acid	201
	propionic acid	202
	butyric acid	203
	isobutyric acid	204
	valeric acid	205
	acrylic acid	206
Aldehydes	formaldehyde	207
	acetaldehyde	208
	propionaldehyde	209
	n-butyraldehyde	210
Ketones	acetone	211
	methyl ethyl ketone	212
	diethyl ketone	213
	methyl isobutyl ketone	214
Ethers	dimethyl ether	215
	methyl ethyl ether	216
	diethyl ether	217
Esters	methyl formate	218
	ethyl formate	219
	n-propyl formate	220
	methyl acetate	221
	vinyl acetate	222
	ethyl acetate	223
	n-propyl acetate	224
	n-butyl acetate	225
	methyl propionate	226
	ethyl propionate	227
	methyl *n*-butyrate	228
	methyl isobutyrate	229
	methyl acrylate	230
	ethyl acrylate	231

	Name of Compound	Selection Number
Amines	methyl amine	232
	dimethyl amine	233
	ethyl amine	234
	ethylenediamine	235
	n-propyl amine	236
	isopropyl amine	237
	trimethyl amine	238
	n-butyl amine	239
	isobutyl amine	240
	diethyl amine	241
	pyridine	242
	aniline	243
	dipropyl amine	244
	triethyl amine	245
	methylphenyl amine	246
	N,N-dimethylaniline	247
	dibutyl amine	248
Nitriles and Other Organo-Nitrogen Compounds	acetonitrile	249
	propionitrile	250
	butyronitrile	251
	nitromethane	252
	ethylene imine	253
Organo-Oxygen Compounds	acrolein	254
	furan	255
	tetrahydrofuran	256
	1,4-dioxane	257
	acetic anhydride	258
Organo-Sulfur Compounds	methyl mercaptan	259
	ethyl mercaptan	260
	dimethyl sulfide	261

Appendix B: Service and Warranty Information

This appendix describes the service provided by Texas Instruments and the warranty for the cartridge.

Table of Contents

Service Information

If you experience a problem with your cartridge, please call or write Consumer Relations to discuss the problem.

For Service and General Information

If you have questions about service or the general use of the cartridge, please call Consumer Relations at:

1-806-747-1882.

Please note that this is a toll number, and collect calls are not accepted.

You may also write to the following address:

Texas Instruments Incorporated
Consumer Relations
P.O. Box 53
Lubbock, Texas 79408

Please contact Consumer Relations:

- Before returning the cartridge for service.
- For general information about using the cartridge.

For Technical Information

If you have technical questions about the operation of the product or programming applications, write to Consumer Relations at the address given above, or call 1-806-741-2663. Please note that this is a toll number, and collect calls are not accepted.

Express Service

Texas Instruments offers an express service option for fast return delivery. Please call Consumer Relations for information.

Calculator Accessories

If you are unable to purchase calculator accessories (such as carrying cases or adapters) from your local dealer, you may order them from Texas Instruments. Please call Consumer Relations for information.

Returning Your Cartridge for Service

A defective cartridge will be either repaired or replaced with the same or comparable reconditioned model (at TI's option) when it is returned, postage prepaid, to a Texas Instruments Service Facility.

Texas Instruments cannot assume responsibility for loss or damage during incoming shipment. For your protection, carefully package the cartridge for shipment and insure it with the carrier. Be sure to enclose the following items with your cartridge:

- Your full return address
- Any accessories related to the problem
- A note describing the problem you experienced
- A copy of your sales receipt or other proof of purchase to determine warranty status

Please ship the cartridge postage prepaid; COD shipments cannot be accepted.

In-Warranty Service

For a cartridge covered under the warranty period, no charge is made for service.

Out-of-Warranty Service

A flat-rate charge by model is made for out-of-warranty service. To obtain the service charge for a particular model, call Consumer Relations **before** returning the product for service. (We cannot hold products in the Service Facility while providing charge information.)

Texas Instruments Service Facilities

U.S. Residents (U.S. Postal Service)
Texas Instruments
P.O. Box 2500
Lubbock, Texas 79408

U.S. Residents (other carriers)
Texas Instruments
2305 N. University
Lubbock, Texas 79415

Canadian Residents Only
Texas Instruments
41 Shelley Road
Richmond Hill, Ontario L4C 5G4

One-Year Limited Warranty

This Texas Instruments software cartridge warranty extends to the original consumer purchaser of the product.

Warranty Duration

This cartridge is warranted to the original consumer purchaser for a period of one (1) year from the original purchase date.

Warranty Coverage

This cartridge is warranted against defective materials or workmanship. **This warranty is void if the product has been damaged by accident, unreasonable use, neglect, improper service, or other causes not arising out of defects in the material or workmanship.**

Warranty Disclaimers

Any implied warranties arising out of this sale, including but not limited to the implied warranties of merchantability and fitness for a particular purpose, are limited in duration to the above one-year period. Texas Instruments shall not be liable for loss of use of the cartridge or other incidental or consequential costs, expenses, or damages incurred by the consumer or any other user.

Some states do not allow the exclusion or limitations of implied warranties or consequential damages, so the above limitations or exclusions may not apply to you.

Legal Remedies

This warranty gives you specific legal rights, and you may also have other rights that vary from state to state.

Warranty Performance

During the above one-year warranty period, your TI cartridge will either be repaired or replaced with a reconditioned comparable model (at TI's option) when the product is returned, postage prepaid, to a Texas Instruments Service Facility.

The repaired or replacement cartridge will be in warranty for the remainder of the original warranty period or for six months, whichever is longer. Other than the postage requirement, no charge will be made for such repair or replacement.

Texas Instruments strongly recommends that you insure the product for value prior to mailing.

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Printed in Taiwan R.O.C.

1061441-0101